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(71) Applicant(s)
F Hoffmann-La Roche AG
(Incorporated in Switzerland)
124 Grenzacherstrasse, CH-4070 Basle,
Switzerland

(72) Inventor(s)
Wendy Lea Corbett
Robert Lewis Crowther
Pete William Dunten
R.Ursula Kammlott
Christine Maria Lukacs

(74) Agent and/or Address for Service
Forrester Ketley & Co
Forrester House, 52 Bounds Green Road,
LONDON, N11 2EY, United Kingdom

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C3H HB7E
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(56) Documents Cited
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Other: ONLINE: WPI, EPODOC, JAPIO,MEDLINE,
BIOSIS, EMBASE, SCISEARCH, CAPLUS

(54) Abstract Title
Crystals of glucokinase and methods of growing them

(57) Crystalline forms of mammalian Glucokinase of sufficient size and quality to obtain structure data by X-ray crystallography are presented. Methods of growing such crystals are also disclosed.
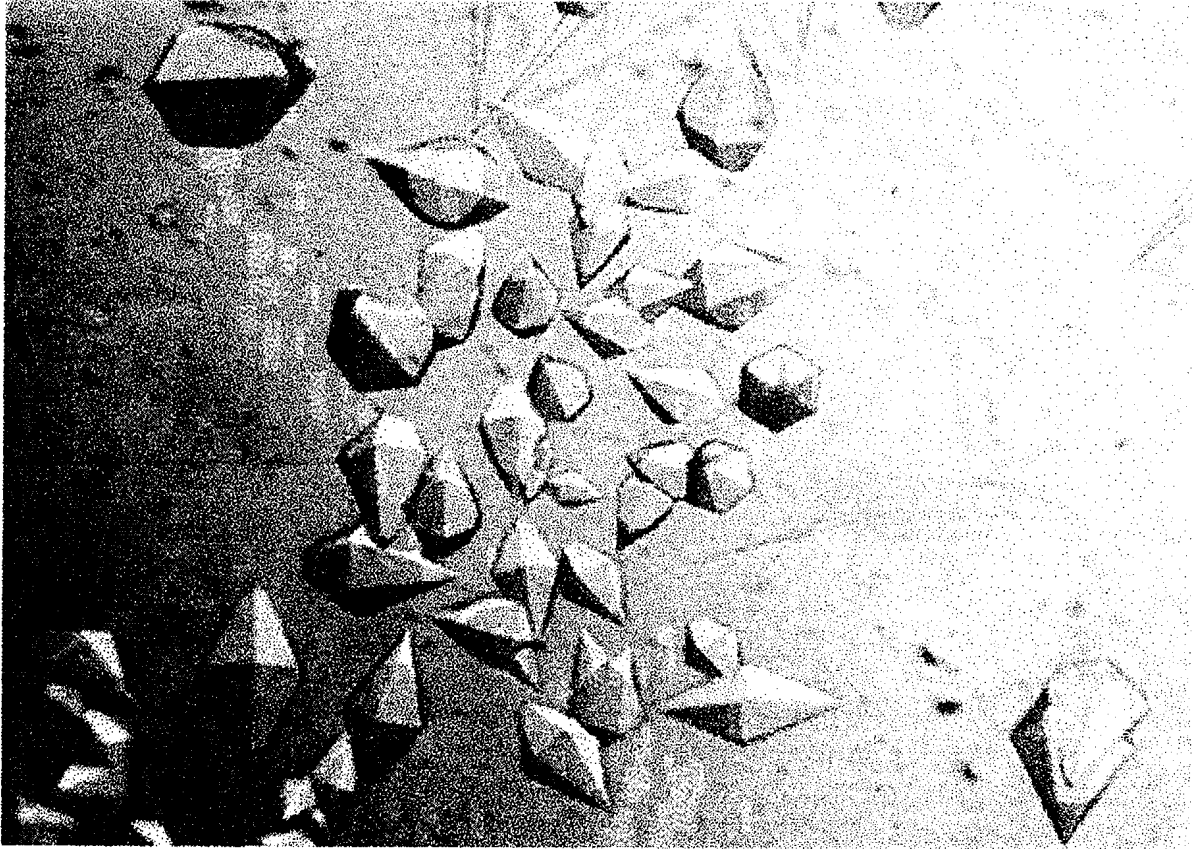
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Figure 1

Figure 2. The amino-acid sequence of the GST-GK fusion protein. The GST sequence was taken from GenBank entry U13852. Residue 229 of the fusion protein is the first residue of GK.

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  1 MSPILGYWKI KGLVQPTRLL LEYLEEKYEE HLYERDEGDK WRNKKFELGL EFPNLPYYID
 61 GDVKLTQSMA IIRYIADKHN MLGGCPKERA EISMLEGAVL DIRYGVSRIA YSKDFETLKV
121 DFLSKLPEML KMFEDRLCHK TYLNGDHVTH PDFMLYDALD VVLYMDPMCL DAFPKLVCFK
181 KRIEAIPQID KYLKSSKYIA WPLQGWQATF GGGDHPPKSD LIEGRGIHMP RPRSQLPQPN
241 SQVEQILAEF QLQEEDLKKV MRRMQKEMDR GLRLETHEEA SVKMLPTYVR STPEGSEVGD
301 FLSLDLGGTN FRVMLVKVGE GEEGQWSVKT KHQMYSIPED AMTGTAEMLF DYISECISDF
361 LDKHQMKHKK LPLGFTFSFP VRHEDIDKGI LLNWTKGFKA SGAEGNNVVG LLRDAIKRRG
421 DFEMDVVAMV NDTVATMISC YYEDHQCEVG MIVGTGCNAC YMEEMQNVEL VEGDEGRMCV
481 NTEWGAFGDS GELDEFLLEY DRLVDESSAN PGQQLYEKLI GGKYMGELVR LVLLRLVDEN
541 LLFHGEASEQ LRTRGAFETR FVSQVESDTG DRKQIYNILS TLGLRPSTTD CDIVRRACES
601 VSTRAAHMCS AGLAGVINRM RESRSEDVMR ITVGVDGSVY KLHPSFKERF HASVRRLTPS
661 CEITFIESEE GSGRGAALVS AVACKKACML GQ
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Figure 3

Figure 4

	Atom No.	Atom Type	A.A. Type	A.A.#	X	Y	Z	OCC	B
	ATOM	1	CB	SER	8	-0.421	63.744	24.899	1.00	50.68
5	ATOM	2	OG	SER	8	-0.752	63.605	23.524	1.00	50.85
	ATOM	3	C	SER	8	1.865	64.216	24.094	1.00	50.72
	ATOM	4	O	SER	8	2.308	63.644	23.102	1.00	51.79
	ATOM	5	N	SER	8	1.473	63.793	26.507	1.00	50.36
	ATOM	6	CA	SER	8	1.057	63.446	25.120	1.00	50.55
10	ATOM	7	N	GLN	9	2.041	65.515	24.314	1.00	49.84
	ATOM	8	CA	GLN	9	2.831	66.312	23.385	1.00	48.95
	ATOM	9	CB	GLN	9	2.983	67.745	23.895	1.00	49.08
	ATOM	10	CG	GLN	9	3.676	68.686	22.925	1.00	50.25
	ATOM	11	CD	GLN	9	3.206	70.127	23.085	1.00	51.06
15	ATOM	12	OE1	GLN	9	2.037	70.433	22.846	1.00	51.38
	ATOM	13	NE2	GLN	9	4.112	71.017	23.499	1.00	51.44
	ATOM	14	C	GLN	9	4.190	65.633	23.294	1.00	48.56
	ATOM	15	O	GLN	9	4.884	65.741	22.285	1.00	48.75
	ATOM	16	N	VAL	10	4.560	64.926	24.361	1.00	47.77
20	ATOM	17	CA	VAL	10	5.823	64.198	24.392	1.00	46.87
	ATOM	18	CB	VAL	10	6.293	63.902	25.842	1.00	46.39
	ATOM	19	CG1	VAL	10	7.303	62.782	25.841	1.00	46.41
	ATOM	20	CG2	VAL	10	6.952	65.135	26.436	1.00	46.79
	ATOM	21	C	VAL	10	5.616	62.885	23.653	1.00	46.17
25	ATOM	22	O	VAL	10	6.521	62.384	22.991	1.00	46.18
	ATOM	23	N	GLU	11	4.423	62.317	23.768	1.00	45.28
	ATOM	24	CA	GLU	11	4.159	61.071	23.069	1.00	45.19
	ATOM	25	CB	GLU	11	2.905	60.393	23.616	1.00	45.21
	ATOM	26	CG	GLU	11	3.105	59.709	24.967	1.00	46.05
30	ATOM	27	CD	GLU	11	4.224	58.664	24.957	1.00	46.30
	ATOM	28	OE1	GLU	11	4.350	57.918	23.948	1.00	46.28
	ATOM	29	OE2	GLU	11	4.963	58.583	25.972	1.00	45.66
	ATOM	30	C	GLU	11	4.002	61.345	21.580	1.00	44.48
	ATOM	31	O	GLU	11	4.068	60.430	20.755	1.00	44.48
35	ATOM	32	N	GLN	12	3.807	62.614	21.239	1.00	43.86
	ATOM	33	CA	GLN	12	3.646	62.996	19.845	1.00	42.86
	ATOM	34	CB	GLN	12	2.972	64.368	19.715	1.00	44.49
	ATOM	35	CG	GLN	12	2.833	64.840	18.259	1.00	46.49
	ATOM	36	CD	GLN	12	1.986	66.099	18.113	1.00	47.74
40	ATOM	37	OE1	GLN	12	2.055	66.799	17.088	1.00	48.30
	ATOM	38	NE2	GLN	12	1.174	66.388	19.131	1.00	47.51
	ATOM	39	C	GLN	12	5.014	63.023	19.192	1.00	41.14
	ATOM	40	O	GLN	12	5.139	62.739	18.002	1.00	41.76
	ATOM	41	N	ILE	13	6.038	63.360	19.971	1.00	38.51
45	ATOM	42	CA	ILE	13	7.398	63.388	19.450	1.00	36.48
	ATOM	43	CB	ILE	13	8.274	64.351	20.261	1.00	35.85
	ATOM	44	CG2	ILE	13	9.731	64.228	19.827	1.00	35.71
	ATOM	45	CG1	ILE	13	7.740	65.777	20.079	1.00	35.77
	ATOM	46	CD1	ILE	13	8.584	66.867	20.710	1.00	35.91
50	ATOM	47	C	ILE	13	8.018	61.981	19.452	1.00	36.01
	ATOM	48	O	ILE	13	8.572	61.528	18.442	1.00	35.99
	ATOM	49	N	LEU	14	7.903	61.288	20.580	1.00	34.88
	ATOM	50	CA	LEU	14	8.430	59.934	20.711	1.00	33.91
	ATOM	51	CB	LEU	14	8.230	59.432	22.141	1.00	33.29
55	ATOM	52	CG	LEU	14	8.853	60.321	23.215	1.00	33.43
	ATOM	53	CD1	LEU	14	8.510	59.781	24.594	1.00	33.04
	ATOM	54	CD2	LEU	14	10.354	60.398	23.001	1.00	33.04

Figure 4

	ATOM	55	C	LEU	14	7.766	58.957	19.730	1.00	33.55	
	ATOM	56	O	LEU	14	8.208	57.812	19.578	1.00	33.21	
	ATOM	57	N	ALA	15	6.710	59.403	19.065	1.00	32.69	
	ATOM	58	CA	ALA	15	6.021	58.551	18.104	1.00	32.59	
5	ATOM	59	CB	ALA	15	4.628	59.104	17.821	1.00	31.95	
	ATOM	60	C	ALA	15	6.838	58.449	16.808	1.00	32.79	
	ATOM	61	O	ALA	15	6.664	57.519	16.018	1.00	33.05	
	ATOM	62	N	GLU	16	7.746	59.395	16.599	1.00	32.33	
	ATOM	63	CA	GLU	16	8.575	59.369	15.403	1.00	32.74	
10	ATOM	64	CB	GLU	16	9.566	60.531	15.401	1.00	34.23	
	ATOM	65	CG	GLU	16	8.950	61.910	15.298	1.00	38.39	
	ATOM	66	CD	GLU	16	10.017	62.998	15.162	1.00	41.11	
	ATOM	67	OE1	GLU	16	10.445	63.269	14.012	1.00	40.68	
	ATOM	68	OE2	GLU	16	10.438	63.562	16.212	1.00	42.77	
15	ATOM	69	C	GLU	16	9.369	58.073	15.279	1.00	31.93	
	ATOM	70	O	GLU	16	9.570	57.568	14.179	1.00	33.41	
	ATOM	71	N	PHE	17	9.841	57.539	16.401	1.00	30.37	
	ATOM	72	CA	PHE	17	10.640	56.321	16.369	1.00	27.71	
	ATOM	73	CB	PHE	17	11.346	56.129	17.711	1.00	26.32	
20	ATOM	74	CG	PHE	17	12.309	57.230	18.045	1.00	24.22	
	ATOM	75	CD1	PHE	17	11.846	58.500	18.389	1.00	23.88	
	ATOM	76	CD2	PHE	17	13.680	57.010	17.981	1.00	22.24	
	ATOM	77	CE1	PHE	17	12.741	59.531	18.660	1.00	22.63	
	ATOM	78	CE2	PHE	17	14.574	58.027	18.250	1.00	21.23	
25	ATOM	79	CZ	PHE	17	14.105	59.291	18.589	1.00	22.01	
	ATOM	80	C	PHE	17	9.836	55. 004	077	16.012	1.00	27.77	27.77
	ATOM	81	O	PHE	17	10.400	54.	15.802	1.00	27.38	
	ATOM	82	N	GLN	18	8.517	55.213	15.957	1.00	28.12	
	ATOM	83	CA	GLN	18	7.684	54.080	15.593	1.00	29.17	
30	ATOM	84	CB	GLN	18	6.216	54.484	15.599	1.00	30.98	
	ATOM	85	CG	GLN	18	5.446	54.017	16.806	1.00	32.94	
	ATOM	86	CD	GLN	18	4.152	54.785	16.974	1.00	34.65	
	ATOM	87	OE1	GLN	18	3.389	54.976	16.014	1.00	37.17	
	ATOM	88	NE2	GLN	18	3.892	55.228	18.190	1.00	33.67	
35	ATOM	89	C	GLN	18	8.068	53.602	14.193	1.00	28.97	
	ATOM	90	O	GLN	18	8.471	54.399	13.346	1.00	28.83	
	ATOM	91	N	LEU	19	7.931	52.298	13.971	1.00	29.02	
	ATOM	92	CA	LEU	19	8.235	51.659	12.704	1.00	29.94	
	ATOM	93	CB	LEU	19	9.641	51.069	12.749	1.00	29.78	
40	ATOM	94	CG	LEU	19	10.782	51.813	12.037	1.00	30.77	
	ATOM	95	CD1	LEU	19	10.886	53.251	12.477	1.00	30.67	
	ATOM	96	CD2	LEU	19	12.083	51.087	12.339	1.00	32.05	
	ATOM	97	C	LEU	19	7.199	50.549	12.511	1.00	31.41	
	ATOM	98	O	LEU	19	7.288	49.484	13.137	1.00	31.35	
45	ATOM	99	N	GLN	20	6.205	50.801	11.663	1.00	32.64	
	ATOM	100	CA	GLN	20	5.153	49.817	11.422	1.00	34.95	
	ATOM	101	CB	GLN	20	4.024	50.413	10.570	1.00	35.78	
	ATOM	102	CG	GLN	20	3.301	51.622	11.175	1.00	37.65	
	ATOM	103	CD	GLN	20	3.048	51.486	12.669	1.00	39.03	
50	ATOM	104	OE1	GLN	20	2.603	50.441	13.152	1.00	40.92	
	ATOM	105	NE2	GLN	20	3.324	52.552	13.410	1.00	40.04	
	ATOM	106	C	GLN	20	5.692	48.568	10.730	1.00	35.83	
	ATOM	107	O	GLN	20	6.827	48.547	10.247	1.00	36.56	
	ATOM	108	N	GLU	21	4.864	47.531	10.681	1.00	36.52	
55	ATOM	109	CA	GLU	21	5.240	46.279	10.062	1.00	37.80	
	ATOM	110	CB	GLU	21	4.024	45.357	9.998	1.00	39.22	
	ATOM	111	CG	GLU	21	4.298	43.898	9.625	1.00	42.88	
	ATOM	112	CD	GLU	21	4.568	43.009	10.844	1.00	44.63	
	ATOM	113	OE1	GLU	21	4.540	41.758	10.699	1.00	45.40	

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	ATOM	114	OE2	GLU	21	4.810	43.564	11.943	1.00	45.89
	ATOM	115	C	GLU	21	5.770	46.549	8.654	1.00	38.20
	ATOM	116	O	GLU	21	6.892	46.183	8.324	1.00	38.71
	ATOM	117	N	GLU	22	4.972	47.208	7.826	1.00	38.54
5	ATOM	118	CA	GLU	22	5.386	47.478	6.457	1.00	39.08
	ATOM	119	CB	GLU	22	4.308	48.267	5.703	1.00	40.61
	ATOM	120	CG	GLU	22	3.123	47.406	5.313	1.00	43.51
	ATOM	121	CD	GLU	22	3.556	46.039	4.773	1.00	45.80
	ATOM	122	OE1	GLU	22	4.243	45.999	3.719	1.00	46.20
10	ATOM	123	OE2	GLU	22	3.215	45.007	5.414	1.00	46.87
	ATOM	124	C	GLU	22	6.711	48.197	6.359	1.00	38.74
	ATOM	125	O	GLU	22	7.482	47.954	5.423	1.00	39.26
	ATOM	126	N	ASP	23	6.988	49.084	7.308	1.00	37.74
	ATOM	127	CA	ASP	23	8.258	49.795	7.276	1.00	37.23
15	ATOM	128	CB	ASP	23	8.356	50.779	8.437	1.00	38.62
	ATOM	129	CG	ASP	23	7.240	51.789	8.427	1.00	40.46
	ATOM	130	OD1	ASP	23	7.104	52.508	7.408	1.00	41.26
	ATOM	131	OD2	ASP	23	6.495	51.861	9.438	1.00	41.77
	ATOM	132	C	ASP	23	9.371	48.760	7.382	1.00	35.54
20	ATOM	133	O	ASP	23	10.267	48.698	6.536	1.00	35.43
	ATOM	134	N	LEU	24	9.294	47.937	8.420	1.00	33.31
	ATOM	135	CA	LEU	24	10.288	46.910	8.631	1.00	32.04
	ATOM	136	CB	LEU	24	9.898	46.062	9.842	1.00	31.35
	ATOM	137	CG	LEU	24	9.920	46.801	11.196	1.00	31.20
25	ATOM	138	CD1	LEU	24	9.710	45.815	12.343	1.00	29.48
	ATOM	139	CD2	LEU	24	11.253	47.526	11.367	1.00	31.51
	ATOM	140	C	LEU	24	10.509	46.041	7.385	1.00	31.61
	ATOM	141	O	LEU	24	11.645	45.723	7.049	1.00	31.67
	ATOM	142	N	LYS	25	9.434	45.673	6.693	1.00	31.58
30	ATOM	143	CA	LYS	25	9.551	44.863	5.486	1.00	31.41
	ATOM	144	CB	LYS	25	8.186	44.347	5.061	1.00	31.91
	ATOM	145	CG	LYS	25	7.574	43.372	6.033	1.00	34.39
	ATOM	146	CD	LYS	25	6.224	42.901	5.531	1.00	36.61
	ATOM	147	CE	LYS	25	5.414	42.232	6.640	1.00	38.71
35	ATOM	148	NZ	LYS	25	3.978	42.086	6.235	1.00	39.39
	ATOM	149	C	LYS	25	10.166	45.679	4.352	1.00	31.50
	ATOM	150	O	LYS	25	10.969	45.170	3.568	1.00	30.92
	ATOM	151	N	LYS	26	9.784	46.947	4.261	1.00	31.82
	ATOM	152	CA	LYS	26	10.332	47.819	3.229	1.00	32.63
40	ATOM	153	CB	LYS	26	9.695	49.203	3.315	1.00	33.38
	ATOM	154	CG	LYS	26	10.053	50.129	2.177	1.00	35.11
	ATOM	155	CD	LYS	26	9.424	51.502	2.400	1.00	37.48
	ATOM	156	CE	LYS	26	9.364	52.312	1.104	1.00	39.72
	ATOM	157	NZ	LYS	26	8.706	53.645	1.307	1.00	42.62
45	ATOM	158	C	LYS	26	11.845	47.919	3.441	1.00	32.91
	ATOM	159	O	LYS	26	12.614	48.012	2.479	1.00	32.90
	ATOM	160	N	VAL	27	12.265	47.901	4.705	1.00	33.16
	ATOM	161	CA	VAL	27	13.687	47.956	5.046	1.00	33.43
	ATOM	162	CB	VAL	27	13.903	48.281	6.555	1.00	32.58
50	ATOM	163	CG1	VAL	27	15.335	47.960	6.963	1.00	32.13
	ATOM	164	CG2	VAL	27	13.622	49.755	6.818	1.00	31.04
	ATOM	165	C	VAL	27	14.305	46.586	4.727	1.00	33.90
	ATOM	166	O	VAL	27	15.323	46.482	4.036	1.00	33.83
	ATOM	167	N	MSE	28	13.668	45.536	5.223	1.00	34.26
55	ATOM	168	CA	MSE	28	14.140	44.193	4.983	1.00	34.84
	ATOM	169	CB	MSE	28	13.072	43.198	5.393	1.00	35.83
	ATOM	170	CG	MSE	28	13.456	41.784	5.144	1.00	38.88
	ATOM	171	SE	MSE	28	12.108	40.670	5.608	1.00	45.40
	ATOM	172	CE	MSE	28	11.054	40.713	4.095	1.00	42.96

Figure 4   7/63

ATOM	173	C	MSE	28	14.465	44.016	3.505	1.00	35.32
ATOM	174	O	MSE	28	15.571	43.621	3.144	1.00	35.22
ATOM	175	N	ARG	29	13.495	44.331	2.655	1.00	36.22
ATOM	176	CA	ARG	29	13.665	44.191	1.218	1.00	36.59
ATOM	177	CB	ARG	29	12.352	44.520	0.509	1.00	37.37
ATOM	178	CG	ARG	29	11.223	43.542	0.827	1.00	38.96
ATOM	179	CD	ARG	29	9.913	43.960	0.152	1.00	40.89
ATOM	180	NE	ARG	29	8.760	43.281	0.744	1.00	42.88
ATOM	181	CZ	ARG	29	7.621	43.889	1.081	1.00	43.80
ATOM	182	NH1	ARG	29	7.475	45.201	0.881	1.00	43.07
ATOM	183	NH2	ARG	29	6.631	43.188	1.636	1.00	44.12
ATOM	184	C	ARG	29	14.814	45.008	0.625	1.00	36.30
ATOM	185	O	ARG	29	15.615	44.469	-0.133	1.00	35.58
ATOM	186	N	ARG	30	14.906	46.296	0.948	1.00	36.85
ATOM	187	CA	ARG	30	16.008	47.091	0.410	1.00	38.41
ATOM	188	CB	ARG	30	15.944	48.543	0.894	1.00	39.31
ATOM	189	CG	ARG	30	14.676	49.285	0.513	1.00	41.96
ATOM	190	CD	ARG	30	14.742	50.763	0.933	1.00	44.07
ATOM	191	NE	ARG	30	13.415	51.384	0.995	1.00	45.48
ATOM	192	CZ	ARG	30	13.179	52.628	1.416	1.00	45.93
ATOM	193	NH1	ARG	30	14.175	53.403	1.810	1.00	45.92
ATOM	194	NH2	ARG	30	11.937	53.091	1.467	1.00	45.68
ATOM	195	C	ARG	30	17.338	46.461	0.843	1.00	39.05
ATOM	196	O	ARG	30	18.286	46.404	0.061	1.00	38.99
ATOM	197	N	MSE	31	17.408	45.999	2.092	1.00	39.11
ATOM	198	CA	MSE	31	18.615	45.348	2.596	1.00	38.96
ATOM	199	CB	MSE	31	18.374	44.784	4.002	1.00	40.43
ATOM	200	CG	MSE	31	19.512	43.922	4.599	1.00	42.62
ATOM	201	SE	MSE	31	21.083	44.819	5.027	1.00	48.46
ATOM	202	CE	MSE	31	20.438	45.988	6.389	1.00	45.46
ATOM	203	C	MSE	31	18.901	44.209	1.633	1.00	38.25
ATOM	204	O	MSE	31	19.973	44.132	1.038	1.00	38.18
ATOM	205	N	GLN	32	17.915	43.334	1.478	1.00	37.93
ATOM	206	CA	GLN	32	18.037	42.199	0.589	1.00	37.33
ATOM	207	CB	GLN	32	16.708	41.475	0.480	1.00	36.41
ATOM	208	CG	GLN	32	16.219	40.905	1.780	1.00	37.04
ATOM	209	CD	GLN	32	15.304	39.723	1.561	1.00	37.28
ATOM	210	OE1	GLN	32	15.740	38.682	1.072	1.00	38.23
ATOM	211	NE2	GLN	32	14.027	39.874	1.912	1.00	37.39
ATOM	212	C	GLN	32	18.475	42.641	-0.791	1.00	37.81
ATOM	213	O	GLN	32	19.215	41.929	-1.466	1.00	37.79
ATOM	214	N	LYS	33	18.019	43.819	-1.205	1.00	38.80
ATOM	215	CA	LYS	33	18.362	44.345	-2.516	1.00	39.85
ATOM	216	CB	LYS	33	17.525	45.588	-2.830	1.00	40.63
ATOM	217	CG	LYS	33	17.591	45.992	-4.298	1.00	42.21
ATOM	218	CD	LYS	33	16.924	47.336	-4.561	1.00	43.78
ATOM	219	CE	LYS	33	17.160	47.803	-6.006	1.00	44.42
ATOM	220	NZ	LYS	33	16.639	49.187	-6.256	1.00	44.23
ATOM	221	C	LYS	33	19.843	44.695	-2.574	1.00	40.37
ATOM	222	O	LYS	33	20.519	44.411	-3.564	1.00	40.53
ATOM	223	N	GLU	34	20.331	45.312	-1.500	1.00	40.59
ATOM	224	CA	GLU	34	21.730	45.712	-1.378	1.00	40.95
ATOM	225	CB	GLU	34	21.912	46.641	-0.179	1.00	41.24
ATOM	226	CG	GLU	34	21.229	47.956	-0.359	1.00	41.42
ATOM	227	CD	GLU	34	21.476	48.506	-1.741	1.00	42.21
ATOM	228	OE1	GLU	34	22.650	48.810	-2.063	1.00	42.30
ATOM	229	OE2	GLU	34	20.493	48.613	-2.507	1.00	43.29
ATOM	230	C	GLU	34	22.667	44.528	-1.221	1.00	40.87
ATOM	231	O	GLU	34	23.770	44.527	-1.767	1.00	41.06

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ATOM	232	N	MSE	35	22.233	43.534	-0.456	1.00	41.15
ATOM	233	CA	MSE	35	23.038	42.350	-0.232	1.00	41.36
ATOM	234	CB	MSE	35	22.289	41.354	0.648	1.00	41.62
ATOM	235	CG	MSE	35	22.320	41.711	2.117	1.00	43.28
ATOM	236	SE	MSE	35	21.428	40.506	3.120	1.00	46.51
ATOM	237	CE	MSE	35	22.217	38.947	2.587	1.00	45.63
ATOM	238	C	MSE	35	23.376	41.701	-1.554	1.00	41.91
ATOM	239	O	MSE	35	24.532	41.367	-1.824	1.00	42.73
ATOM	240	N	ASP	36	22.367	41.533	-2.395	1.00	42.15
ATOM	241	CA	ASP	36	22.593	40.898	-3.675	1.00	41.96
ATOM	242	CB	ASP	36	21.264	40.633	-4.369	1.00	43.56
ATOM	243	CG	ASP	36	21.446	39.947	-5.699	1.00	45.91
ATOM	244	OD1	ASP	36	21.821	40.652	-6.675	1.00	46.71
ATOM	245	OD2	ASP	36	21.232	38.707	-5.754	1.00	46.76
ATOM	246	C	ASP	36	23.502	41.717	-4.578	1.00	41.03
ATOM	247	O	ASP	36	24.406	41.178	-5.217	1.00	40.61
ATOM	248	N	ARG	37	23.257	43.021	-4.620	1.00	40.36
ATOM	249	CA	ARG	37	24.034	43.937	-5.446	1.00	39.76
ATOM	250	CB	ARG	37	23.498	45.355	-5.283	1.00	39.56
ATOM	251	CG	ARG	37	22.252	45.621	-6.112	1.00	40.04
ATOM	252	CD	ARG	37	21.465	46.815	-5.590	1.00	41.19
ATOM	253	NE	ARG	37	22.278	48.002	-5.307	1.00	41.70
ATOM	254	CZ	ARG	37	22.938	48.711	-6.221	1.00	42.38
ATOM	255	NH1	ARG	37	22.899	48.362	-7.505	1.00	42.59
ATOM	256	NH2	ARG	37	23.615	49.792	-5.851	1.00	41.94
ATOM	257	C	ARG	37	25.524	43.908	-5.152	1.00	39.94
ATOM	258	O	ARG	37	26.335	43.732	-6.059	1.00	40.39
ATOM	259	N	GLY	38	25.893	44.076	-3.890	1.00	39.94
ATOM	260	CA	GLY	38	27.305	44.063	-3.557	1.00	39.60
ATOM	261	C	GLY	38	27.933	42.689	-3.699	1.00	39.23
ATOM	262	O	GLY	38	29.163	42.546	-3.695	1.00	39.59
ATOM	263	N	LEU	39	27.087	41.677	-3.834	1.00	38.16
ATOM	264	CA	LEU	39	27.545	40.307	-3.960	1.00	37.65
ATOM	265	CB	LEU	39	26.428	39.376	-3.495	1.00	35.76
ATOM	266	CG	LEU	39	26.821	38.029	-2.900	1.00	34.52
ATOM	267	CD1	LEU	39	27.899	38.248	-1.857	1.00	33.52
ATOM	268	CD2	LEU	39	25.606	37.348	-2.284	1.00	32.44
ATOM	269	C	LEU	39	27.931	39.989	-5.407	1.00	39.20
ATOM	270	O	LEU	39	28.594	38.980	-5.681	1.00	39.88
ATOM	271	N	ARG	40	27.537	40.866	-6.329	1.00	40.51
ATOM	272	CA	ARG	40	27.809	40.656	-7.751	1.00	41.77
ATOM	273	CB	ARG	40	26.494	40.686	-8.526	1.00	42.80
ATOM	274	CG	ARG	40	25.735	39.392	-8.377	1.00	44.75
ATOM	275	CD	ARG	40	24.257	39.551	-8.636	1.00	46.47
ATOM	276	NE	ARG	40	23.639	38.239	-8.797	1.00	48.71
ATOM	277	CZ	ARG	40	22.331	38.034	-8.890	1.00	50.01
ATOM	278	NH1	ARG	40	21.497	39.064	-8.831	1.00	51.43
ATOM	279	NH2	ARG	40	21.861	36.804	-9.060	1.00	50.46
ATOM	280	C	ARG	40	28.802	41.623	-8.374	1.00	42.16
ATOM	281	O	ARG	40	28.783	42.819	-8.097	1.00	42.42
ATOM	282	N	LEU	41	29.650	41.087	-9.247	1.00	42.03
ATOM	283	CA	LEU	41	30.689	41.864	-9.902	1.00	42.00
ATOM	284	CB	LEU	41	31.307	41.044	-11.041	1.00	42.00
ATOM	285	CG	LEU	41	32.577	41.650	-11.660	1.00	41.78
ATOM	286	CD1	LEU	41	33.638	41.836	-10.583	1.00	40.20
ATOM	287	CD2	LEU	41	33.087	40.747	-12.773	1.00	41.95
ATOM	288	C	LEU	41	30.278	43.237	-10.428	1.00	42.57
ATOM	289	O	LEU	41	30.920	44.243	-10.110	1.00	42.64
ATOM	290	N	GLU	42	29.219	43.292	-11.227	1.00	43.03

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	ATOM	291	CA	GLU	42	28.788	44.562	-11.803	1.00 44.63
	ATOM	292	CB	GLU	42	27.494	44.369	-12.607	1.00 43.97
	ATOM	293	CG	GLU	42	26.436	43.533	-11.922	1.00 44.02
	ATOM	294	CD	GLU	42	26.546	42.057	-12.248	1.00 43.71
5	ATOM	295	OE1	GLU	42	27.673	41.527	-12.245	1.00 45.13
	ATOM	296	OE2	GLU	42	25.504	41.416	-12.496	1.00 43.50
	ATOM	297	C	GLU	42	28.616	45.714	-10.805	1.00 46.21
	ATOM	298	O	GLU	42	28.963	46.860	-11.103	1.00 46.22
	ATOM	299	N	THR	43	28.105	45.413	-9.616	1.00 47.90
10	ATOM	300	CA	THR	43	27.873	46.443	-8.608	1.00 49.10
	ATOM	301	CB	THR	43	26.370	46.533	-8.285	1.00 48.63
	ATOM	302	OG1	THR	43	25.772	45.242	-8.465	1.00 47.66
	ATOM	303	CG2	THR	43	25.679	47.531	-9.192	1.00 48.90
	ATOM	304	C	THR	43	28.629	46.226	-7.302	1.00 50.94
15	ATOM	305	O	THR	43	28.481	47.008	-6.362	1.00 51.52
	ATOM	306	N	HIS	44	29.456	45.185	-7.249	1.00 52.58
	ATOM	307	CA	HIS	44	30.204	44.854	-6.037	1.00 53.89
	ATOM	308	CB	HIS	44	31.210	43.727	-6.311	1.00 54.68
	ATOM	309	CG	HIS	44	32.552	44.208	-6.775	1.00 55.77
20	ATOM	310	CD2	HIS	44	33.748	44.257	-6.139	1.00 55.82
	ATOM	311	ND1	HIS	44	32.758	44.772	-8.017	1.00 56.36
	ATOM	312	CE1	HIS	44	34.020	45.146	-8.125	1.00 56.30
	ATOM	313	NE2	HIS	44	34.643	44.845	-6.999	1.00 56.06
	ATOM	314	C	HIS	44	30.950	46.013	-5.398	1.00 54.87
25	ATOM	315	O	HIS	44	30.823	46.254	-4.199	1.00 55.06
	ATOM	316	N	GLU	45	31.724	46.732	-6.203	1.00 56.25
	ATOM	317	CA	GLU	45	32.540	47.826	-5.703	1.00 57.17
	ATOM	318	CB	GLU	45	33.618	48.180	-6.721	1.00 59.35
	ATOM	319	CG	GLU	45	33.146	49.127	-7.800	1.00 61.61
30	ATOM	320	CD	GLU	45	34.107	50.279	-7.985	1.00 63.07
	ATOM	321	OE1	GLU	45	35.228	50.038	-8.487	1.00 63.72
	ATOM	322	OE2	GLU	45	33.747	51.420	-7.613	1.00 64.00
	ATOM	323	C	GLU	45	31.762	49.074	-5.356	1.00 56.66
	ATOM	324	O	GLU	45	32.295	49.985	-4.732	1.00 56.54
35	ATOM	325	N	GLU	46	30.508	49.135	-5.772	1.00 56.24
	ATOM	326	CA	GLU	46	29.708	50.306	-5.456	1.00 56.37
	ATOM	327	CB	GLU	46	29.542	51.157	-6.704	1.00 57.92
	ATOM	328	CG	GLU	46	30.881	51.645	-7.212	1.00 60.77
	ATOM	329	CD	GLU	46	30.782	52.400	-8.515	1.00 62.28
40	ATOM	330	OE1	GLU	46	30.566	51.762	-9.571	1.00 62.25
	ATOM	331	OE2	GLU	46	30.914	53.641	-8.474	1.00 63.95
	ATOM	332	C	GLU	46	28.366	49.891	-4.873	1.00 55.40
	ATOM	333	O	GLU	46	27.309	50.123	-5.457	1.00 55.75
	ATOM	334	N	ALA	47	28.440	49.264	-3.704	1.00 53.89
45	ATOM	335	CA	ALA	47	27.273	48.783	-2.987	1.00 51.80
	ATOM	336	CB	ALA	47	27.140	47.280	-3.159	1.00 52.36
	ATOM	337	C	ALA	47	27.470	49.111	-1.524	1.00 49.98
	ATOM	338	O	ALA	47	28.448	48.664	-0.923	1.00 50.36
	ATOM	339	N	SER	48	26.553	49.894	-0.960	1.00 47.18
50	ATOM	340	CA	SER	48	26.630	50.267	0.444	1.00 44.70
	ATOM	341	CB	SER	48	25.299	50.860	0.897	1.00 46.13
	ATOM	342	OG	SER	48	24.243	49.927	0.720	1.00 47.87
	ATOM	343	C	SER	48	26.965	49.041	1.287	1.00 42.45
	ATOM	344	O	SER	48	27.841	49.082	2.147	1.00 42.01
55	ATOM	345	N	VAL	49	26.261	47.946	1.037	1.00 40.48
	ATOM	346	CA	VAL	49	26.516	46.713	1.762	1.00 38.96
	ATOM	347	CB	VAL	49	25.231	45.849	1.875	1.00 38.62
	ATOM	348	CG1	VAL	49	25.496	44.625	2.740	1.00 38.40
	ATOM	349	CG2	VAL	49	24.102	46.672	2.472	1.00 37.16

Figure 4

	ATOM	350	C	VAL	49	27.572	45.997	0.929	1.00	37.97
	ATOM	351	O	VAL	49	27.266	45.474	-0.137	1.00	38.42
	ATOM	352	N	LYS	50	28.810	45.982	1.422	1.00	36.51
	ATOM	353	CA	LYS	50	29.937	45.385	0.703	1.00	34.95
5	ATOM	354	CB	LYS	50	31.250	45.843	1.334	1.00	35.51
	ATOM	355	CG	LYS	50	31.574	47.322	1.091	1.00	36.68
	ATOM	356	CD	LYS	50	30.676	48.249	1.913	1.00	39.05
	ATOM	357	CE	LYS	50	30.865	48.018	3.419	1.00	39.54
	ATOM	358	NZ	LYS	50	32.316	48.157	3.792	1.00	40.04
10	ATOM	359	C	LYS	50	30.012	43.879	0.482	1.00	33.72
	ATOM	360	O	LYS	50	30.845	43.421	-0.293	1.00	33.30
	ATOM	361	N	MSE	51	29.171	43.100	1.147	1.00	33.02
	ATOM	362	CA	MSE	51	29.209	41.647	0.967	1.00	32.08
	ATOM	363	CB	MSE	51	28.291	41.257	-0.190	1.00	34.01
15	ATOM	364	CG	MSE	51	26.867	41.744	-0.025	1.00	36.03
	ATOM	365	SE	MSE	51	26.148	41.146	1.529	1.00	40.73
	ATOM	366	CE	MSE	51	25.558	39.411	1.085	1.00	37.98
	ATOM	367	C	MSE	51	30.637	41.180	0.666	1.00	30.17
	ATOM	368	O	MSE	51	30.928	40.723	-0.437	1.00	30.22
20	ATOM	369	N	LEU	52	31.518	41.295	1.650	1.00	28.96
	ATOM	370	CA	LEU	52	32.920	40.928	1.487	1.00	27.43
	ATOM	371	CB	LEU	52	33.769	41.839	2.357	1.00	28.05
	ATOM	372	CG	LEU	52	33.649	43.319	1.991	1.00	28.52
	ATOM	373	CD1	LEU	52	34.222	44.171	3.116	1.00	28.77
25	ATOM	374	CD2	LEU	52	34.369	43.583	0.658	1.00	28.75
	ATOM	375	C	LEU	52	33.273	39.482	1.803	1.00	26.61
	ATOM	376	O	LEU	52	32.997	38.995	2.893	1.00	25.26
	ATOM	377	N	PRO	53	33.911	38.774	0.844	1.00	27.04
	ATOM	378	CD	PRO	53	34.270	39.142	-0.540	1.00	25.69
30	ATOM	379	CA	PRO	53	34.264	37.375	1.133	1.00	27.99
	ATOM	380	CB	PRO	53	34.807	36.864	-0.204	1.00	26.92
	ATOM	381	CG	PRO	53	34.184	37.825	-1.241	1.00	25.77
	ATOM	382	C	PRO	53	35.314	37.361	2.239	1.00	28.40
	ATOM	383	O	PRO	53	36.152	38.271	2.317	1.00	28.36
35	ATOM	384	N	THR	54	35.255	36.329	3.080	1.00	29.46
	ATOM	385	CA	THR	54	36.149	36.142	4.226	1.00	30.53
	ATOM	386	CB	THR	54	35.317	35.951	5.502	1.00	29.48
	ATOM	387	OG1	THR	54	34.589	34.711	5.418	1.00	27.97
	ATOM	388	CG2	THR	54	34.324	37.084	5.659	1.00	29.42
40	ATOM	389	C	THR	54	37.018	34.884	4.071	1.00	31.60
	ATOM	390	O	THR	54	37.657	34.423	5.025	1.00	32.25
	ATOM	391	N	TYR	55	37.017	34.311	2.877	1.00	32.63
	ATOM	392	CA	TYR	55	37.763	33.089	2.615	1.00	34.41
	ATOM	393	CB	TYR	55	39.249	33.421	2.405	1.00	33.07
45	ATOM	394	CG	TYR	55	39.458	34.175	1.101	1.00	32.58
	ATOM	395	CD1	TYR	55	39.518	35.571	1.067	1.00	32.44
	ATOM	396	CE1	TYR	55	39.572	36.263	-0.157	1.00	32.48
	ATOM	397	CD2	TYR	55	39.467	33.492	-0.117	1.00	31.97
	ATOM	398	CE2	TYR	55	39.516	34.172	-1.335	1.00	31.83
50	ATOM	399	CZ	TYR	55	39.566	35.548	-1.351	1.00	32.18
	ATOM	400	OH	TYR	55	39.575	36.200	-2.568	1.00	32.67
	ATOM	401	C	TYR	55	37.559	31.956	3.637	1.00	36.06
	ATOM	402	O	TYR	55	38.314	30.991	3.665	1.00	37.61
	ATOM	403	N	VAL	56	36.518	32.059	4.459	1.00	38.03
55	ATOM	404	CA	VAL	56	36.199	31.006	5.429	1.00	39.87
	ATOM	405	CB	VAL	56	35.483	31.586	6.663	1.00	38.75
	ATOM	406	CG1	VAL	56	35.202	30.492	7.669	1.00	38.10
	ATOM	407	CG2	VAL	56	36.336	32.660	7.285	1.00	38.76
	ATOM	408	C	VAL	56	35.249	30.032	4.706	1.00	42.20

Figure 4

	ATOM	409	O	VAL	56	34.098	30.376	4.418	1.00	42.02
	ATOM	410	N	ARG	57	35.718	28.821	4.414	1.00	44.49
	ATOM	411	CA	ARG	57	34.896	27.860	3.676	1.00	47.07
	ATOM	412	CB	ARG	57	35.688	27.288	2.499	1.00	48.02
5	ATOM	413	CG	ARG	57	36.209	28.310	1.508	1.00	49.08
	ATOM	414	CD	ARG	57	36.558	27.626	0.185	1.00	49.69
	ATOM	415	NE	ARG	57	37.239	28.528	-0.737	1.00	49.50
	ATOM	416	CZ	ARG	57	38.367	29.167	-0.447	1.00	48.83
	ATOM	417	NH1	ARG	57	38.938	28.997	0.745	1.00	48.13
10	ATOM	418	NH2	ARG	57	38.915	29.978	-1.345	1.00	47.51
	ATOM	419	C	ARG	57	34.311	26.695	4.449	1.00	48.57
	ATOM	420	O	ARG	57	34.810	26.310	5.500	1.00	48.65
	ATOM	421	N	SER	58	33.256	26.117	3.891	1.00	51.15
	ATOM	422	CA	SER	58	32.589	24.973	4.501	1.00	54.78
15	ATOM	423	CB	SER	58	31.204	24.793	3.882	1.00	54.26
	ATOM	424	OG	SER	58	31.258	24.980	2.475	1.00	54.39
	ATOM	425	C	SER	58	33.419	23.708	4.295	1.00	57.39
	ATOM	426	O	SER	58	33.097	22.645	4.823	1.00	57.47
	ATOM	427	N	THR	59	34.484	23.840	3.510	1.00	60.71
20	ATOM	428	CA	THR	59	35.392	22.740	3.216	1.00	64.02
	ATOM	429	CB	THR	59	35.886	22.823	1.758	1.00	63.73
	ATOM	430	OG1	THR	59	36.637	24.029	1.570	1.00	63.22
	ATOM	431	CG2	THR	59	34.704	22.843	0.801	1.00	63.87
	ATOM	432	C	THR	59	36.571	22.880	4.176	1.00	67.10
25	ATOM	433	O	THR	59	37.554	23.562	3.884	1.00	67.44
	ATOM	434	N	PRO	60	36.480	22.238	5.349	1.00	69.75
	ATOM	435	CD	PRO	60	35.366	21.412	5.854	1.00	70.63
	ATOM	436	CA	PRO	60	37.556	22.320	6.337	1.00	71.72
	ATOM	437	CB	PRO	60	36.841	21.982	7.636	1.00	71.72
30	ATOM	438	CG	PRO	60	35.909	20.881	7.182	1.00	71.50
	ATOM	439	C	PRO	60	38.709	21.370	6.056	1.00	73.48
	ATOM	440	O	PRO	60	39.522	21.609	5.158	1.00	73.53
	ATOM	441	N	GLU	61	38.754	20.287	6.830	1.00	75.48
	ATOM	442	CA	GLU	61	39.808	19.283	6.731	1.00	76.98
35	ATOM	443	CB	GLU	61	39.969	18.788	5.289	1.00	78.43
	ATOM	444	CG	GLU	61	40.806	17.516	5.161	1.00	80.68
	ATOM	445	CD	GLU	61	42.177	17.744	4.530	1.00	81.88
	ATOM	446	OE1	GLU	61	42.993	18.498	5.100	1.00	82.28
	ATOM	447	OE2	GLU	61	42.442	17.156	3.458	1.00	82.68
40	ATOM	448	C	GLU	61	41.083	19.969	7.194	1.00	77.00
	ATOM	449	O	GLU	61	41.942	20.327	6.389	1.00	77.10
	ATOM	450	N	GLY	62	41.177	20.181	8.502	1.00	76.85
	ATOM	451	CA	GLY	62	42.344	20.826	9.069	1.00	76.72
	ATOM	452	C	GLY	62	42.415	20.539	10.555	1.00	76.65
45	ATOM	453	O	GLY	62	42.507	19.380	10.969	1.00	76.79
	ATOM	454	N	SER	63	42.361	21.594	11.362	1.00	76.25
	ATOM	455	CA	SER	63	42.417	21.458	12.814	1.00	75.06
	ATOM	456	CB	SER	63	41.401	20.413	13.300	1.00	75.92
	ATOM	457	OG	SER	63	41.350	20.363	14.718	1.00	76.69
50	ATOM	458	C	SER	63	43.818	21.062	13.259	1.00	73.60
	ATOM	459	O	SER	63	44.090	19.899	13.561	1.00	73.10
	ATOM	460	N	GLU	64	44.705	22.045	13.280	1.00	71.83
	ATOM	461	CA	GLU	64	46.071	21.819	13.703	1.00	70.12
	ATOM	462	CB	GLU	64	46.996	22.824	13.011	1.00	71.42
55	ATOM	463	CG	GLU	64	48.464	22.726	13.417	1.00	73.74
	ATOM	464	CD	GLU	64	49.014	21.309	13.342	1.00	74.84
	ATOM	465	OE1	GLU	64	48.623	20.466	14.187	1.00	75.26
	ATOM	466	OE2	GLU	64	49.837	21.041	12.434	1.00	75.45
	ATOM	467	C	GLU	64	46.136	21.971	15.221	1.00	67.97

Figure 4 12/63

	ATOM	468	O	GLU	64	46.775	22.886	15.734	1.00	68.33
	ATOM	469	N	VAL	65	45.448	21.076	15.927	1.00	65.13
	ATOM	470	CA	VAL	65	45.400	21.067	17.391	1.00	62.32
	ATOM	471	CB	VAL	65	45.335	19.621	17.918	1.00	62.48
5	ATOM	472	CG1	VAL	65	45.487	19.607	19.430	1.00	62.45
	ATOM	473	CG2	VAL	65	44.011	18.975	17.508	1.00	62.79
	ATOM	474	C	VAL	65	46.587	21.752	18.055	1.00	60.42
	ATOM	475	O	VAL	65	47.703	21.708	17.540	1.00	60.54
	ATOM	476	N	GLY	66	46.354	22.386	19.200	1.00	58.26
10	ATOM	477	CA	GLY	66	47.454	23.043	19.888	1.00	55.67
	ATOM	478	C	GLY	66	47.081	24.174	20.823	1.00	53.42
	ATOM	479	O	GLY	66	46.153	24.052	21.615	1.00	54.08
	ATOM	480	N	ASP	67	47.832	25.267	20.739	1.00	51.06
	ATOM	481	CA	ASP	67	47.614	26.460	21.549	1.00	48.67
15	ATOM	482	CB	ASP	67	48.617	26.531	22.703	1.00	49.14
	ATOM	483	CG	ASP	67	48.381	25.462	23.751	1.00	49.34
	ATOM	484	OD1	ASP	67	48.201	24.287	23.365	1.00	49.37
	ATOM	485	OD2	ASP	67	48.386	25.791	24.956	1.00	49.62
	ATOM	486	C	ASP	67	47.832	27.634	20.612	1.00	47.26
20	ATOM	487	O	ASP	67	48.786	27.635	19.827	1.00	47.44
	ATOM	488	N	PHE	68	46.955	28.632	20.678	1.00	45.41
	ATOM	489	CA	PHE	68	47.075	29.778	19.785	1.00	43.60
	ATOM	490	CB	PHE	68	46.031	29.682	18.667	1.00	41.17
	ATOM	491	CG	PHE	68	46.032	28.361	17.946	1.00	39.29
25	ATOM	492	CD1	PHE	68	45.621	27.199	18.592	1.00	38.55
	ATOM	493	CD2	PHE	68	46.468	28.272	16.623	1.00	38.76
	ATOM	494	CE1	PHE	68	45.647	25.966	17.934	1.00	38.24
	ATOM	495	CE2	PHE	68	46.498	27.050	15.959	1.00	37.31
	ATOM	496	CZ	PHE	68	46.086	25.893	16.619	1.00	37.76
30	ATOM	497	C	PHE	68	46.918	31.096	20.514	1.00	43.33
	ATOM	498	O	PHE	68	46.395	31.147	21.621	1.00	43.27
	ATOM	499	N	LEU	69	47.386	32.166	19.889	1.00	43.51
	ATOM	500	CA	LEU	69	47.274	33.475	20.497	1.00	44.73
	ATOM	501	CB	LEU	69	48.625	34.197	20.518	1.00	45.26
35	ATOM	502	CG	LEU	69	48.781	34.949	21.848	1.00	46.33
	ATOM	503	CD1	LEU	69	49.166	33.928	22.932	1.00	46.09
	ATOM	504	CD2	LEU	69	49.811	36.072	21.748	1.00	45.48
	ATOM	505	C	LEU	69	46.275	34.278	19.681	1.00	45.37
	ATOM	506	O	LEU	69	46.448	34.451	18.470	1.00	45.62
40	ATOM	507	N	SER	70	45.228	34.758	20.351	1.00	45.75
	ATOM	508	CA	SER	70	44.177	35.528	19.697	1.00	44.98
	ATOM	509	CB	SER	70	42.794	34.984	20.074	1.00	44.61
	ATOM	510	OG	SER	70	42.697	33.589	19.844	1.00	44.25
	ATOM	511	C	SER	70	44.250	36.978	20.109	1.00	44.92
45	ATOM	512	O	SER	70	44.451	37.289	21.277	1.00	44.67
	ATOM	513	N	LEU	71	44.095	37.858	19.130	1.00	45.85
	ATOM	514	CA	LEU	71	44.092	39.294	19.366	1.00	47.27
	ATOM	515	CB	LEU	71	45.064	40.000	18.421	1.00	47.71
	ATOM	516	CG	LEU	71	46.552	39.942	18.787	1.00	49.06
50	ATOM	517	CD1	LEU	71	47.008	38.497	19.039	1.00	49.69
	ATOM	518	CD2	LEU	71	47.348	40.572	17.656	1.00	49.35
	ATOM	519	C	LEU	71	42.668	39.752	19.082	1.00	47.94
	ATOM	520	O	LEU	71	41.873	38.997	18.499	1.00	48.06
	ATOM	521	N	ASP	72	42.333	40.976	19.479	1.00	48.20
55	ATOM	522	CA	ASP	72	40.985	41.451	19.244	1.00	48.67
	ATOM	523	CB	ASP	72	40.043	40.807	20.262	1.00	48.71
	ATOM	524	CG	ASP	72	38.668	41.420	20.243	1.00	49.13
	ATOM	525	OD1	ASP	72	38.090	41.549	19.144	1.00	49.57
	ATOM	526	OD2	ASP	72	38.168	41.777	21.331	1.00	50.11

Figure 4

	ATOM	527	C	ASP	72	40.819	42.962	19.258	1.00	48.98
	ATOM	528	O	ASP	72	40.247	43.530	20.187 ·	1.00	48.82
	ATOM	529	N	LEU	73	41.312	43.613	18.214	1.00	49.73
	ATOM	530	CA	LEU	73	41.193	45.060	18.117	1.00	51.48
5	ATOM	531	CB	LEU	73	42.199	45.603	17.096	1.00	50.80
	ATOM	532	CG	LEU	73	42.160	47.096	16.774	1.00	50.07
	ATOM	533	CD1	LEU	73	42.358	47.902	18.045	1.00	50.10
	ATOM	534	CD2	LEU	73	43.223	47.421	15.738	1.00	49.97
	ATOM	535	C	LEU	73	39.764	45.392	17.687	1.00	52.93
10	ATOM	536	O	LEU	73	38.909	44.507	17.628	1.00	52.38
	ATOM	537	N	GLY	74	39.504	46.665	17.401	1.00	54.88
	ATOM	538	CA	GLY	74	38.177	47.068	16.983	1.00	56.88
	ATOM	539	C	GLY	74	37.285	47.420	18.148	1.00	58.48
	ATOM	540	O	GLY	74	36.476	48.348	18.071	1.00	58.31
15	ATOM	541	N	GLY	75	37.428	46.668	19.233	1.00	60.27
	ATOM	542	CA	GLY	75	36.621	46.925	20.410	1.00	62.46
	ATOM	543	C	GLY	75	37.020	48.230	21.074	1.00	63.75
	ATOM	544	O	GLY	75	37.824	49.005	20.536	1.00	64.06
	ATOM	545	N	THR	76	36.452	48.481	22.248	1.00	64.50
20	ATOM	546	CA	THR	76	36.759	49.697	22.991	1.00	65.42
	ATOM	547	CB	THR	76	35.905	49.776	24.266	1.00	66.28
	ATOM	548	OG1	THR	76	36.361	48.791	25.203	1.00	67.43
	ATOM	549	CG2	THR	76	34.425	49.505	23.938	1.00	66.14
	ATOM	550	C	THR	76	38.238	49.651	23.385	1.00	65.25
25	ATOM	551	O	THR	76	39.005	50.595	23.152	1.00	65.01
	ATOM	552	N	ASN	77	38.622	48.528	23.980	1.00	64.74
	ATOM	553	CA	ASN	77	39.987	48.309	24.412	1.00	64.17
	ATOM	554	CB	ASN	77	40.015	47.966	25.903	1.00	65.44
	ATOM	555	CG	ASN	77	39.346	49.027	26.765	1.00	66.47
30	ATOM	556	OD1	ASN	77	39.656	50.219	26.663	1.00	67.13
	ATOM	557	ND2	ASN	77	38.431	48.596	27.629	1.00	66.65
	ATOM	558	C	ASN	77	40.547	47.149	23.603	1.00	63.19
	ATOM	559	O	ASN	77	39.795	46.303	23.120	1.00	62.58
	ATOM	560	N	PHE	78	41.866	47.123	23.446	1.00	62.14
35	ATOM	561	CA	PHE	78	42.526	46.051	22.708	1.00	61.12
	ATOM	562	CB	PHE	78	43.887	46.514	22.172	1.00	61.81
	ATOM	563	CG	PHE	78	44.684	45.420	21.516	1.00	62.50
	ATOM	564	CD1	PHE	78	44.347	44.956	20.245	1.00	62.81
	ATOM	565	CD2	PHE	78	45.741	44.818	22.189	1.00	62.99
40	ATOM	566	CE1	PHE	78	45.051	43.899	19.655	1.00	62.72
	ATOM	567	CE2	PHE	78	46.450	43.763	21.607	1.00	63.38
	ATOM	568	CZ	PHE	78	46.103	43.301	20.336	1.00	63.01
	ATOM	569	C	PHE	78	42.732	44.893	23.668	1.00	60.09
	ATOM	570	O	PHE	78	43.065	45.100	24.834	1.00	60.08
45	ATOM	571	N	ARG	79	42.528	43.675	23.184	1.00	58.63
	ATOM	572	CA	ARG	79	42.706	42.504	24.025	1.00	57.40
	ATOM	573	CB	ARG	79	41.367	41.819	24.280	1.00	57.06
	ATOM	574	CG	ARG	79	41.481	40.637	25.222	1.00	57.49
	ATOM	575	CD	ARG	79	40.221	39.819	25.219	1.00	57.47
50	ATOM	576	NE	ARG	79	39.062	40.646	25.504	1.00	57.16
	ATOM	577	CZ	ARG	79	37.818	40.266	25.267	1.00	57.69
	ATOM	578	NH1	ARG	79	37.586	39.071	24.738	1.00	57.38
	ATOM	579	NH2	ARG	79	36.812	41.080	25.555	1.00	58.45
	ATOM	580	C	ARG	79	43.663	41.522	23.368	1.00	56.71
55	ATOM	581	O	ARG	79	43.926	41.619	22.170	1.00	57.24
	ATOM	582	N	VAL	80	44.180	40.590	24.167	1.00	55.50
	ATOM	583	CA	VAL	80	45.114	39.557	23.724	1.00	54.27
	ATOM	584	CB	VAL	80	46.576	39.947	23.996	1.00	54.31
	ATOM	585	CG1	VAL	80	47.491	38.779	23.674	1.00	54.49

Figure 4 14/63

	ATOM	586	CG2	VAL	80	46.960	41.158	23.166	1.00	54.39
	ATOM	587	C	VAL	80	44.806	38.327	24.555	1.00	54.04
	ATOM	588	O	VAL	80	44.517	38.447	25.738	1.00	53.31
	ATOM	589	N	MSE	81	44.881	37.144	23.957	1.00	54.52
5	ATOM	590	CA	MSE	81	44.568	35.935	24.703	1.00	54.59
	ATOM	591	CB	MSE	81	43.053	35.804	24.828	1.00	57.08
	ATOM	592	CG	MSE	81	42.300	36.025	23.520	1.00	60.39
	ATOM	593	SE	MSE	81	40.534	36.437	23.792	1.00	65.62
	ATOM	594	CE	MSE	81	39.999	34.926	24.679	1.00	62.03
10	ATOM	595	C	MSE	81	45.142	34.645	24.146	1.00	53.56
	ATOM	596	O	MSE	81	45.598	34.582	23.007	1.00	52.99
	ATOM	597	N	LEU	82	45.096	33.611	24.978	1.00	52.63
	ATOM	598	CA	LEU	82	45.602	32.292	24.638	1.00	51.86
	ATOM	599	CB	LEU	82	46.660	31.863	25.665	1.00	52.75
15	ATOM	600	CG	LEU	82	47.261	30.455	25.542	1.00	53.22
	ATOM	601	CD1	LEU	82	48.562	30.521	24.736	1.00	52.42
	ATOM	602	CD2	LEU	82	47.523	29.882	26.937	1.00	53.00
	ATOM	603	C	LEU	82	44.461	31.286	24.650	1.00	51.18
	ATOM	604	O	LEU	82	43.718	31.186	25.632	1.00	51.20
20	ATOM	605	N	VAL	83	44.333	30.535	23.563	1.00	50.58
	ATOM	606	CA	VAL	83	43.292	29.522	23.448	1.00	50.00
	ATOM	607	CB	VAL	83	42.274	29.887	22.362	1.00	49.63
	ATOM	608	CG1	VAL	83	41.213	28.794	22.262	1.00	49.26
	ATOM	609	CG2	VAL	83	41.660	31.244	22.670	1.00	48.32
25	ATOM	610	C	VAL	83	43.914	28.187	23.080	1.00	50.53
	ATOM	611	O	VAL	83	44.759	28.122	22.192	1.00	50.93
	ATOM	612	N	LYS	84	43.496	27.127	23.763	1.00	51.05
	ATOM	613	CA	LYS	84	44.017	25.788	23.504	1.00	51.89
	ATOM	614	CB	LYS	84	44.338	25.061	24.826	1.00	51.79
30	ATOM	615	CG	LYS	84	44.716	23.581	24.659	1.00	51.85
	ATOM	616	CD	LYS	84	44.951	22.870	26.009	1.00	51.58
	ATOM	617	CE	LYS	84	46.429	22.848	26.422	1.00	50.92
	ATOM	618	NZ	LYS	84	47.041	24.198	26.592	1.00	50.33
	ATOM	619	C	LYS	84	42.997	24.983	22.708	1.00	52.68
35	ATOM	620	O	LYS	84	42.115	24.327	23.282	1.00	53.00
	ATOM	621	N	VAL	85	43.124	25.038	21.383	1.00	52.91
	ATOM	622	CA	VAL	85	42.224	24.319	20.488	1.00	52.70
	ATOM	623	CB	VAL	85	42.399	24.805	19.048	1.00	51.79
	ATOM	624	CG1	VAL	85	41.302	24.232	18.176	1.00	52.19
40	ATOM	625	CG2	VAL	85	42.389	26.319	19.017	1.00	51.59
	ATOM	626	C	VAL	85	42.525	22.823	20.548	1.00	53.51
	ATOM	627	O	VAL	85	43.637	22.389	20.243	1.00	53.87
	ATOM	628	N	GLY	86	41.534	22.037	20.952	1.00	54.38
	ATOM	629	CA	GLY	86	41.726	20.603	21.053	1.00	55.35
45	ATOM	630	C	GLY	86	40.901	19.810	20.060	1.00	56.21
	ATOM	631	O	GLY	86	40.136	20.370	19.278	1.00	55.63
	ATOM	632	N	GLU	87	41.050	18.493	20.106	1.00	57.81
	ATOM	633	CA	GLU	87	40.339	17.611	19.195	1.00	59.64
	ATOM	634	CB	GLU	87	41.290	16.529	18.673	1.00	60.88
50	ATOM	635	CG	GLU	87	40.680	15.648	17.611	1.00	62.26
	ATOM	636	CD	GLU	87	40.215	16.457	16.423	1.00	63.21
	ATOM	637	OE1	GLU	87	41.072	16.931	15.644	1.00	63.20
	ATOM	638	OE2	GLU	87	38.989	16.631	16.278	1.00	64.58
	ATOM	639	C	GLU	87	39.133	16.959	19.859	1.00	60.12
55	ATOM	640	O	GLU	87	39.271	16.187	20.810	1.00	60.00
	ATOM	641	N	GLY	88	37.948	17.273	19.347	1.00	60.93
	ATOM	642	CA	GLY	88	36.735	16.707	19.902	1.00	61.61
	ATOM	643	C	GLY	88	35.840	16.120	18.833	1.00	62.11
	ATOM	644	O	GLY	88	36.038	16.346	17.638	1.00	61.67

Figure 4 15/63

	ATOM	645	N	GLU	89	34.845	15.363	19.274	1.00 62.79
	ATOM	646	CA	GLU	89	33.898	14.724	18.372	1.00 63.90
	ATOM	647	CB	GLU	89	32.782	14.089	19.203	1.00 63.50
	ATOM	648	CG	GLU	89	33.304	13.137	20.275	1.00 62.64
5	ATOM	649	CD	GLU	89	32.214	12.623	21.203	1.00 62.46
	ATOM	650	OE1	GLU	89	32.510	11.728	22.019	1.00 62.39
	ATOM	651	OE2	GLU	89	31.064	13.110	21.128	1.00 62.11
	ATOM	652	C	GLU	89	33.312	15.688	17.325	1.00 65.16
	ATOM	653	O	GLU	89	32.975	16.837	17.634	1.00 64.98
10	ATOM	654	N	GLU	90	33.204	15.205	16.087	1.00 66.03
	ATOM	655	CA	GLU	90	32.667	15.977	14.958	1.00 66.67
	ATOM	656	CB	GLU	90	31.135	15.974	14.978	1.00 67.21
	ATOM	657	CG	GLU	90	30.495	14.620	14.717	1.00 66.83
	ATOM	658	CD	GLU	90	28.986	14.662	14.869	1.00 67.49
15	ATOM	659	OE1	GLU	90	28.308	15.273	14.009	1.00 67.±7
	ATOM	660	OE2	GLU	90	28.480	14.090	15.858	1.00 66.84
	ATOM	661	C	GLU	90	33.149	17.421	14.871	1.00 66.91
	ATOM	662	O	GLU	90	32.623	18.212	14.080	1.00 66.74
	ATOM	663	N	GLY	91	34.149	17.769	15.671	1.00 67.05
20	ATOM	664	CA	GLY	91	34.649	19.126	15.628	1.00 67.38
	ATOM	665	C	GLY	91	36.036	19.339	16.201	1.00 67.42
	ATOM	666	O	GLY	91	37.025	18.797	15.708	1.00 68.24
	ATOM	667	N	GLN	92	36.094	20.154	17.246	1.00 66.86
	ATOM	668	CA	GLN	92	37.335	20.492	17.929	1.00 65.93
25	ATOM	669	CB	GLN	92	38.395	20.968	16.924	1.00 66.17
	ATOM	670	CG	GLN	92	38.007	22.215	16.159	1.00 66.24
	ATOM	671	CD	GLN	92	38.564	22.236	14.750	1.00 66.57
	ATOM	672	OE1	GLN	92	38.432	21.260	14.007	1.00 66.37
	ATOM	673	NE2	GLN	92	39.177	23.356	14.367	1.00 66.54
30	ATOM	674	C	GLN	92	36.999	21.605	18.920	1.00 65.21
	ATOM	675	O	GLN	92	36.625	22.721	18.530	1.00 65.44
	ATOM	676	N	TRP	93	37.111	21.278	20.204	1.00 63.62
	ATOM	677	CA	TRP	93	36.820	22.227	21.261	1.00 61.61
	ATOM	678	CB	TRP	93	36.859	21.540	22.626	1.00 62.77
35	ATOM	679	CG	TRP	93	38.050	20.641	22.857	1.00 63.86
	ATOM	680	CD2	TRP	93	39.213	20.943	23.637	1.00 64.17
	ATOM	681	CE2	TRP	93	40.026	19.787	23.645	1.00 64.21
	ATOM	682	CE3	TRP	93	39.647	22.080	24.336	1.00 64.11
	ATOM	683	CD1	TRP	93	38.206	19.349	22.424	1.00 63.84
40	ATOM	684	NE1	TRP	93	39.387	18.830	22.897	1.00 63.69
	ATOM	685	CZ2	TRP	93	41.246	19.731	24.324	1.00 64.43
	ATOM	686	CZ3	TRP	93	40.859	22.026	25.009	1.00 64.63
	ATOM	687	CH2	TRP	93	41.645	20.857	24.999	1.00 64.71
	ATOM	688	C	TRP	93	37.784	23.393	21.248	1.00 59.53
45	ATOM	689	O	TRP	93	38.733	23.420	20.474	1.00 59.18
	ATOM	690	N	SER	94	37.521	24.366	22.106	1.00 57.94
	ATOM	691	CA	SER	94	38.353	25.549	22.207	1.00 56.46
	ATOM	692	CB	SER	94	37.880	26.615	21.219	1.00 56.58
	ATOM	693	OG	SER	94	36.504	26.899	21.412	1.00 56.78
50	ATOM	694	C	SER	94	38.185	26.050	23.624	1.00 55.56
	ATOM	695	O	SER	94	37.142	25.822	24.237	1.00 55.36
	ATOM	696	N	VAL	95	39.208	26.722	24.146	1.00 54.53
	ATOM	697	CA	VAL	95	39.152	27.248	25.504	1.00 53.17
	ATOM	698	CB	VAL	95	39.511	26.183	26.549	1.00 52.17
55	ATOM	699	CG1	VAL	95	39.742	26.844	27.891	1.00 52.13
	ATOM	700	CG2	VAL	95	38.396	25.172	26.666	1.00 51.73
	ATOM	701	C	VAL	95	40.099	28.399	25.719	1.00 52.74
	ATOM	702	O	VAL	95	41.268	28.315	25.357	1.00 53.14
	ATOM	703	N	LYS	96	39.587	29.469	26.318	1.00 52.63

Figure 4 16/63

	ATOM	704	CA	LYS	96	40.402	30.637	26.629	1.00	52.93
	ATOM	705	CB	LYS	96	39.513	31.849	26.932	1.00	53.25
	ATOM	706	CG	LYS	96	40.277	33.129	27.231	1.00	53.79
	ATOM	707	CD	LYS	96	39.910	33.706	28.595	1.00	54.80
5	ATOM	708	CE	LYS	96	38.427	34.102	28.682	1.00	55.69
	ATOM	709	NZ	LYS	96	38.027	35.162	27.696	1.00	55.59
	ATOM	·710	C	LYS	96	41.154	30.218	27.882	1.00	52.96
	ATOM	711	O	LYS	96	40.546	29.733	28.834	1.00	52.93
	ATOM	712	N	THR	97	42.470	30.384	27.886	1.00	53.38
10	ATOM	713	CA	THR	97	43.253	29.980	29.050	1.00	53.93
	ATOM	714	CB	THR	97	44.238	28.850	28.684	1.00	53.99
	ATOM	715	OG1	THR	97	43.512	27.736	28.151	1.00	52.99
	ATOM	716	CG2	THR	97	44.998	28.394	29.918	1.00	55.29
	ATOM	717	C	THR	97	44.036	31.132	29.670	1.00	53.82
15	ATOM	718	O	THR	97	44.330	31.123	30.866	1.00	53.54
	ATOM	719	N	LYS	98	44.373	32.117	28.848	1.00	53.85
	ATOM	720	CA	LYS	98	45.115	33.276	29.315	1.00	54.60
	ATOM	721	CB	LYS	98	46.627	33.096	29.087	1.00	55.51
	ATOM	722	CG	LYS	98	47.220	31.809	29.652	1.00	56.78
20	ATOM	723	CD	LYS	98	47.074	31.733	31.162	1.00	58.23
	ATOM	724	CE	LYS	98	47.553	30.389	31.713	1.00	58.82
	ATOM	725	NZ	LYS	98	47.404	30.320	33.201	1.00	58.98
	ATOM	726	C	LYS	98	44.644	34.479	28.518	1.00	54.54
	ATOM	727	O	LYS	98	44.323	34.360	27.329	1.00	54.79
25	ATOM	728	N	HIS	99	44.590	35.632	29.173	1.00	54.03
	ATOM	729	CA	HIS	99	44.193	36.853	28.496	1.00	54.03
	ATOM	730	CB	HIS	99	42.720	36.793	28.052	1.00	55.02
	ATOM	731	CG	HIS	99	41.732	36.872	29.172	1.00	55.71
	ATOM	732	CD2	HIS	99	40.682	37.704	29.373	1.00	55.66
30	ATOM	733	ND1	HIS	99	41.739	35.999	30.239	1.00	56.19
	ATOM	734	CE1	HIS	99	40.736	36.288	31.049	1.00	56.30
	ATOM	735	NE2	HIS	99	40.080	37.319	30.546	1.00	56.72
	ATOM	736	C	HIS	99	44.445	38.082	29.351	1.00	53.46
	ATOM	737	O	HIS	99	44.526	38.007	30.577	1.00	53.47
35	ATOM	738	N	GLN	100	44.583	39.214	28.683	1.00	52.94
	ATOM	739	CA	GLN	100	44.841	40.468	29.349	1.00	53.34
	ATOM	740	CB	GLN	100	46.354	40.649	29.513	1.00	53.39
	ATOM	741	CG	GLN	100	46.790	42.001	30.055	1.00	54.26
	ATOM	742	CD	GLN	100	46.168	42.345	31.394	1.00	54.43
40	ATOM	743	OE1	GLN	100	46.349	41.629	32.384	1.00	55.27
	ATOM	744	NE2	GLN	100	45.433	43.452	31.432	1.00	53.60
	ATOM	745	C	GLN	100	44.243	41.567	28.481	1.00	53.43
	ATOM	746	O	GLN	100	44.416	41.569	27.260	1.00	53.75
	ATOM	747	N	THR	101	43.527	42.493	29.105	1.00	52.90
45	ATOM	748	CA	THR	101	42.905	43.576	28.367	1.00	53.12
	ATOM	749	CB	THR	101	41.495	43.826	28.894	1.00	52.52
	ATOM	750	OG1	THR	101	40.789	42.582	28.925	1.00	52.85
	ATOM	751	CG2	THR	101	40.752	44.808	27.999	1.00	52.23
	ATOM	752	C	THR	101	43.731	44.845	28.499	1.00	53.61
50	ATOM	753	O	THR	101	44.285	45.108	29.563	1.00	53.95
	ATOM	754	N	TYR	102	43.809	45.628	27.422	1.00	54.10
	ATOM	755	CA	TYR	102	44.585	46.869	27.422	1.00	55.36
	ATOM	756	CB	TYR	102	45.878	46.708	26.608	1.00	54.89
	ATOM	757	CG	TYR	102	46.788	45.569	27.015	1.00	54.25
55	ATOM	758	CD1	TYR	102	46.382	44.241	26.888	1.00	54.08
	ATOM	759	CE1	TYR	102	47.227	43.197	27.226	1.00	53.44
	ATOM	760	CD2	TYR	102	48.069	45.822	27.497	1.00	53.79
	ATOM	761	CE2	TYR	102	48.922	44.785	27.840	1.00	53.76
	ATOM	762	CZ	TYR	102	48.498	43.475	27.701	1.00	53.85

Figure 4 17/63

	ATOM	763	OH	TYR	102	49.355	42.442	28.021	1.00	54.03
	ATOM	764	C	TYR	102	43.813	48.041	26.822	1.00	56.65
	ATOM	765	O	TYR	102	43.173	47.899	25.781	1.00	56.91
	ATOM	766	N	SER	103	43.891	49.203	27.462	1.00	58.50
5	ATOM	767	CA	SER	103	43.217	50.385	26.938	1.00	60.94
	ATOM	768	CB	SER	103	42.997	51.411	28.049	1.00	61.09
	ATOM	769	OG	SER	103	44.231	51.829	28.602	1.00	62.50
	ATOM	770	C	SER	103	44.090	50.985	25.833	1.00	62.31
	ATOM	771	O	SER	103	45.293	50.729	25.771	1.00	62.27
10	ATOM	772	N	ALA	104	43.487	51.783	24.960	1.00	64.47
	ATOM	773	CA	ALA	104	44.226	52.386	23.856	1.00	67.01
	ATOM	774	CB	ALA	104	43.516	52.093	22.526	1.00	67.01
	ATOM	775	C	ALA	104	44.410	53.888	24.025	1.00	68.66
	ATOM	776	O	ALA	104	43.458	54.658	23.902	1.00	69.01
15	ATOM	777	N	PRO	105	45.648	54.327	24.305	1.00	70.09
	ATOM	778	CD	PRO	105	46.878	53.522	24.397	1.00	70.06
	ATOM	779	CA	PRO	105	45.946	55.751	24.485	1.00	71.25
	ATOM	780	CB	PRO	105	47.443	55.748	24.783	1.00	70.79
	ATOM	781	CG	PRO	105	47.929	54.535	24.046	1.00	70.54
20	ATOM	782	C	PRO	105	45.592	56.586	23.251	1.00	72.81
	ATOM	783	O	PRO	105	45.837	56.170	22.117	1.00	73.09
	ATOM	784	N	GLU	106	45.012	57.762	23.479	1.00	74.39
	ATOM	785	CA	GLU	106	44.619	58.652	22.391	1.00	76.25
	ATOM	786	CB	GLU	106	43.991	59.921	22.950	1.00	76.77
25	ATOM	787	CG	GLU	106	42.702	59.673	23.680	1.00	78.35
	ATOM	788	CD	GLU	106	42.397	60.775	24.657	1.00	79.28
	ATOM	789	OE1	GLU	106	42.239	61.934	24.214	1.00	79.74
	ATOM	790	OE2	GLU	106	42.326	60.478	25.871	1.00	80.03
	ATOM	791	C	GLU	106	45.784	59.028	21.494	1.00	77.33
30	ATOM	792	O	GLU	106	45.600	59.262	20.300	1.00	77.48
	ATOM	793	N	ASP	107	46.980	59.104	22.068	1.00	78.72
	ATOM	794	CA	ASP	107	48.161	59.440	21.284	1.00	80.10
	ATOM	795	CB	ASP	107	49.431	59.316	22.134	1.00	80.44
	ATOM	796	CG	ASP	107	49.965	57.889	22.185	1.00	81.03
35	ATOM	797	OD1	ASP	107	49.198	56.976	22.569	1.00	81.42
	ATOM	798	OD2	ASP	107	51.151	57.682	21.839	1.00	80.86
	ATOM	799	C	ASP	107	48.212	58.424	20.151	1.00	80.92
	ATOM	800	O	ASP	107	48.724	58.703	19.065	1.00	81.29
	ATOM	801	N	ALA	108	47.670	57.241	20.428	1.00	81.68
40	ATOM	802	CA	ALA	108	47.628	56.151	19.463	1.00	82.45
	ATOM	803	CB	ALA	108	47.605	54.813	20.200	1.00	82.45
	ATOM	804	C	ALA	108	46.406	56.275	18.553	1.00	82.91
	ATOM	805	O	ALA	108	46.536	56.351	17.331	1.00	82.98
	ATOM	806	N	MSE	109	45.221	56.303	19.157	1.00	83.41
45	ATOM	807	CA	MSE	109	43.974	56.414	18.407	1.00	83.78
	ATOM	808	CB	MSE	109	42.787	56.519	19.368	1.00	85.45
	ATOM	809	CG	MSE	109	41.581	55.678	18.972	1.00	87.01
	ATOM	810	SE	MSE	109	41.933	53.898	19.096	1.00	90.12
	ATOM	811	CE	MSE	109	42.665	53.581	17.453	1.00	88.95
50	ATOM	812	C	MSE	109	43.992	57.633	17.494	1.00	83.17
	ATOM	813	O	MSE	109	43.235	57.710	16.527	1.00	83.19
	ATOM	814	N	THR	110	44.854	58.590	17.820	1.00	82.51
	ATOM	815	CA	THR	110	44.986	59.815	17.040	1.00	82.00
	ATOM	816	CB	THR	110	45.289	61.022	17.949	1.00	82.44
55	ATOM	817	OG1	THR	110	44.302	61.103	18.986	1.00	83.00
	ATOM	818	CG2	THR	110	45.283	62.313	17.142	1.00	82.69
	ATOM	819	C	THR	110	46.150	59.640	16.082	1.00	81.25
	ATOM	820	O	THR	110	46.127	60.123	14.949	1.00	80.95
	ATOM	821	N	GLY	111	47.168	58.933	16.559	1.00	80.84

Figure 4

	ATOM	822	CA	GLY	111	48.358	58.691	15.768	1.00	80.12
	ATOM	823	C	GLY	111	48.121	57.986	14.450	1.00	79.53
	ATOM	824	O	GLY	111	47.018	57.531	14.148	1.00	79.54
	ATOM	825	N	THR	112	49.181	57.904	13.658	1.00	78.87
5	ATOM	826	CA	THR	112	49.129	57.254	12.360	1.00	78.09
	ATOM	827	CB	THR	112	50.427	57.553	11.561	1.00	78.67
	ATOM	828	OG1	THR	112	50.329	57.001	10.240	1.00	79.18
	ATOM	829	CG2	THR	112	51.644	56.956	12.279	1.00	78.48
	ATOM	830	C	THR	112	48.992	55.748	12.579	1.00	77.09
10	ATOM	831	O	THR	112	49.231	55.254	13.685	1.00	76.48
	ATOM	832	N	ALA	113	48.601	55.027	11.529	1.00	76.26
	ATOM	833	CA	ALA	113	48.443	53.573	11.603	1.00	75.60
	ATOM	834	CB	ALA	113	48.184	53.001	10.208	1.00	76.00
	ATOM	835	C	ALA	113	49.711	52.965	12.191	1.00	74.65
15	ATOM	836	O	ALA	113	49.665	52.006	12.968	1.00	74.58
	ATOM	837	N	GLU	114	50.845	53.538	11.803	1.00	73.24
	ATOM	838	CA	GLU	114	52.139	53.088	12.288	1.00	71.57
	ATOM	839	CB	GLU	114	53.246	53.971	11.700	1.00	72.34
	ATOM	840	CG	GLU	114	53.130	54.167	10.188	1.00	71.64
20	ATOM	841	CD	GLU	114	53.325	52.877	9.401	1.00	72.49
	ATOM	842	OE1	GLU	114	53.192	51.781	9.994	1.00	72.24
	ATOM	843	OE2	GLU	114	53.600	52.960	8.183	1.00	71.83
	ATOM	844	C	GLU	114	52.085	53.233	13.801	1.00	70.37
	ATOM	845	O	GLU	114	52.297	52.266	14.537	1.00	69.92
25	ATOM	846	N	MET	115	51.778	54.450	14.246	1.00	68.75
	ATOM	847	CA	MET	115	51.657	54.760	15.669	1.00	66.97
	ATOM	848	CB	MET	115	51.013	56.140	15.866	1.00	67.15
	ATOM	849	CG	MET	115	51.999	57.277	16.040	1.00	66.94
	ATOM	850	SD	MET	115	53.203	56.869	17.320	1.00	67.61
30	ATOM	851	CE	MET	115	52.137	56.732	18.788	1.00	66.65
	ATOM	852	C	MET	115	50.799	53.718	16.374	1.00	65.81
	ATOM	853	O	MET	115	51.266	53.010	17.275	1.00	65.94
	ATOM	854	N	LEU	116	49.542	53.635	15.940	1.00	63.70
	ATOM	855	CA	LEU	116	48.561	52.711	16.504	1.00	61.63
35	ATOM	856	CB	LEU	116	47.287	52.720	15.650	1.00	60.89
	ATOM	857	CG	LEU	116	45.948	52.226	16.205	1.00	59.42
	ATOM	858	CD1	LEU	116	44.953	52.182	15.051	1.00	58.84
	ATOM	859	CD2	LEU	116	46.081	50.858	16.847	1.00	58.86
	ATOM	860	C	LEU	116	49.083	51.285	16.613	1.00	60.35
40	ATOM	861	O	LEU	116	48.977	50.665	17.667	1.00	60.48
	ATOM	862	N	PHE	117	49.641	50.756	15.531	1.00	59.14
	ATOM	863	CA	PHE	117	50.138	49.391	15.580	1.00	58.14
	ATOM	864	CB	PHE	117	50.298	48.819	14.173	1.00	57.03
	ATOM	865	CG	PHE	117	49.055	48.144	13.669	1.00	56.22
45	ATOM	866	CD1	PHE	117	48.005	48.889	13.143	1.00	55.49
	ATOM	867	CD2	PHE	117	48.909	46.763	13.783	1.00	55.59
	ATOM	868	CE1	PHE	117	46.830	48.270	12.741	1.00	55.25
	ATOM	869	CE2	PHE	117	47.736	46.134	13.384	1.00	55.20
	ATOM	870	CZ	PHE	117	46.695	46.887	12.862	1.00	55.23
50	ATOM	871	C	PHE	117	51.415	49.204	16.382	1.00	57.89
	ATOM	872	O	PHE	117	51.799	48.073	16.690	1.00	57.80
	ATOM	873	N	ALA	118	52.078	50.303	16.725	1.00	57.35
	ATOM	874	CA	ALA	118	53.275	50.193	17.537	1.00	56.79
	ATOM	875	CB	ALA	118	54.004	51.533	17.594	1.00	56.42
55	ATOM	876	C	ALA	118	52.747	49.792	18.922	1.00	56.46
	ATOM	877	O	ALA	118	53.220	48.829	19.536	1.00	56.68
	ATOM	878	N	ALA	119	51.733	50.515	19.391	1.00	55.57
	ATOM	879	CA	ALA	119	51.142	50.226	20.693	1.00	55.05
	ATOM	880	CB	ALA	119	49.931	51.135	20.952	1.00	53.91

Figure 4 19/63

	ATOM	881	C	ALA	119	50.719	48.769	20.763	1.00	54.96
	ATOM	882	O	ALA	119	51.090	48.052	21.698	1.00	54.94
	ATOM	883	N	ILE	120	49.948	48.338	19.763	1.00	55.10
	ATOM	884	CA	ILE	120	49.443	46.969	19.715	1.00	55.51
5	ATOM	885	CB	ILE	120	48.679	46.679	18.397	1.00	54.45
	ATOM	886	CG2	ILE	120	47.922	45.363	18.525	1.00	53.30
	ATOM	887	CG1	ILE	120	47.688	47.808	18.089	1.00	53.32
	ATOM	888	CD1	ILE	120	46.871	47.581	16.820	1.00	51.70
	ATOM	889	C	ILE	120	50.575	45.957	19.846	1.00	56.57
10	ATOM	890	O	ILE	120	50.477	45.006	20.632	1.00	56.52
	ATOM	891	N	SER	121	51.645	46.169	19.076	1.00	57.78
	ATOM	892	CA	SER	121	52.814	45.284	19.093	1.00	58.54
	ATOM	893	CB	SER	121	53.844	45.730	18.045	1.00	58.96
	ATOM	894	OG	SER	121	53.377	45.507	16.720	1.00	59.32
15	ATOM	895	C	SER	121	53.457	45.280	20.473	1.00	58.74
	ATOM	896	O	SER	121	54.007	44.265	20.918	1.00	57.56
	ATOM	897	N	GLU	122	53.379	46.422	21.151	1.00	59.50
	ATOM	898	CA	GLU	122	53.947	46.529	22.484	1.00	60.44
	ATOM	899	CB	GLU	122	54.003	47.986	22.941	1.00	60.60
20	ATOM	900	CG	GLU	122	55.104	48.241	23.952	1.00	60.45
	ATOM	901	CD	GLU	122	54.706	49.252	25.003	1.00	61.76
	ATOM	902	OE1	GLU	122	54.152	50.312	24.630	1.00	61.92
	ATOM	903	OE2	GLU	122	54.950	48.986	26.202	1.00	62.20
	ATOM	904	C	GLU	122	53.091	45.725	23.452	1.00	60.63
25	ATOM	905	O	GLU	122	53.565	44.761	24.048	1.00	60.82
	ATOM	906	N	CYS	123	51.831	46.120	23.605	1.00	60.96
	ATOM	907	CA	CYS	123	50.936	45.410	24.510	1.00	61.79
	ATOM	908	CB	CYS	123	49.481	45.840	24.278	1.00	61.63
	ATOM	909	SG	CYS	123	49.191	47.636	24.439	1.00	62.83
30	ATOM	910	C	CYS	123	51.107	43.922	24.233	1.00	61.90
	ATOM	911	O	CYS	123	51.028	43.095	25.147	1.00	61.89
	ATOM	912	N	ILE	124	51.350	43.588	22.966	1.00	62.36
	ATOM	913	CA	ILE	124	51.561	42.197	22.588	1.00	62.79
	ATOM	914	CB	ILE	124	52.033	42.061	21.109	1.00	62.52
35	ATOM	915	CG2	ILE	124	52.618	40.676	20.877	1.00	61.07
	ATOM	916	CG1	ILE	124	50.866	42.280	20.138	1.00	61.53
	ATOM	917	CD1	ILE	124	50.016	41.038	19.888	1.00	61.77
	ATOM	918	C	ILE	124	52.673	41.706	23.499	1.00	62.76
	ATOM	919	O	ILE	124	52.475	40.807	24.320	1.00	62.23
40	ATOM	920	N	SER	125	53.839	42.327	23.347	1.00	63.43
	ATOM	921	CA	SER	125	55.020	42.002	24.138	1.00	64.63
	ATOM	922	CB	SER	125	56.062	43.117	23.986	1.00	65.05
	ATOM	923	OG	SER	125	57.324	42.745	24.523	1.00	67.01
	ATOM	924	C	SER	125	54.646	41.840	25.610	1.00	64.32
45	ATOM	925	O	SER	125	54.886	40.794	26.219	1.00	64.46
	ATOM	926	N	ASP	126	54.047	42.884	26.169	1.00	64.43
	ATOM	927	CA	ASP	126	53.626	42.894	27.562	1.00	64.86
	ATOM	928	CB	ASP	126	52.660	44.060	27.788	1.00	64.95
	ATOM	929	CG	ASP	126	52.390	44.323	29.253	1.00	65.38
50	ATOM	930	OD1	ASP	126	51.952	43.389	29.955	1.00	65.74
	ATOM	931	OD2	ASP	126	52.613	45.467	29.706	1.00	65.92
	ATOM	932	C	ASP	126	52.968	41.572	27.980	1.00	64.65
	ATOM	933	O	ASP	126	53.424	40.918	28.924	1.00	64.28
	ATOM	934	N	PHE	127	51.902	41.189	27.274	1.00	64.96
55	ATOM	935	CA	PHE	127	51.177	39.948	27.565	1.00	65.21
	ATOM	936	CB	PHE	127	50.145	39.657	26.468	1.00	64.22
	ATOM	937	CG	PHE	127	49.569	38.258	26.525	1.00	63.67
	ATOM	938	CD1	PHE	127	48.774	37.857	27.594	1.00	63.64
	ATOM	939	CD2	PHE	127	49.830	37.343	25.512	1.00	63.42

Figure 4

	ATOM	940	CE1	PHE	127	48.247	36.564	27.652	1.00	63.40
	ATOM	941	CE2	PHE	127	49.308	36.051	25.560	1.00	63.55
	ATOM	942	CZ	PHE	127	48.516	35.661	26.632	1.00	63.49
	ATOM	943	C	PHE	127	52.154	38.791	27.631	1.00	65.83
5	ATOM	944	O	PHE	127	52.195	38.030	28.600	1.00	65.71
	ATOM	945	N	LEU	128	52.931	38.684	26.562	1.00	66.57
	ATOM	946	CA	LEU	128	53.942	37.656	26.387	1.00	67.52
	ATOM	947	CB	LEU	128	54.773	38.022	25.166	1.00	67.64
	ATOM	948	CG	LEU	128	53.926	38.452	23.969	1.00	67.42
10	ATOM	949	CD1	LEU	128	54.819	39.108	22.941	1.00	67.90
	ATOM	950	CD2	LEU	128	53.195	37.251	23.387	1.00	67.65
	ATOM	951	C	LEU	128	54.850	37.502	27.609	1.00	68.09
	ATOM	952	O	LEU	128	54.829	36.468	28.285	1.00	67.92
	ATOM	953	N	ASP	129	55.654	38.530	27.878	1.00	68.62
15	ATOM	954	CA	ASP	129	56.565	38.514	29.018	1.00	69.22
	ATOM	955	CB	ASP	129	57.135	39.907	29.287	1.00	68.93
	ATOM	956	CG	ASP	129	58.115	40.342	28.239	1.00	68.90
	ATOM	957	OD1	ASP	129	59.100	39.606	28.011	1.00	69.12
	ATOM	958	OD2	ASP	129	57.900	41.423	27.650	1.00	69.22
20	ATOM	959	C	ASP	129	55.843	38.059	30.267	1.00	69.59
	ATOM	960	O	ASP	129	56.063	36.956	30.761	1.00	69.41
	ATOM	961	N	LYS	130	54.973	38.940	30.753	1.00	70.10
	ATOM	962	CA	LYS	130	54.190	38.733	31.958	1.00	70.67
	ATOM	963	CB	LYS	130	53.285	39.946	32.159	1.00	70.80
25	ATOM	964	CG	LYS	130	54.076	41.252	32.052	1.00	70.54
	ATOM	965	CD	LYS	130	53.218	42.479	32.266	1.00	70.22
	ATOM	966	CE	LYS	130	54.021	43.746	32.011	1.00	70.07
	ATOM	967	NZ	LYS	130	53.204	44.977	32.195	1.00	69.69
	ATOM	968	C	LYS	130	53.394	37.441	31.982	1.00	71.17
30	ATOM	969	O	LYS	130	52.381	37.331	32.673	1.00	70.99
	ATOM	970	N	HIS	131	53.883	36.468	31.221	1.00	72.01
	ATOM	971	CA	HIS	131	53.301	35.139	31.125	1.00	73.44
	ATOM	972	CB	HIS	131	52.313	35.065	29.965	1.00	73.00
	ATOM	973	CG	HIS	131	50.881	35.076	30.397	1.00	72.93
35	ATOM	974	CD2	HIS	131	49.960	34.085	30.454	1.00	72.73
	ATOM	975	ND1	HIS	131	50.256	36.210	30.869	1.00	72.87
	ATOM	976	CE1	HIS	131	49.010	35.917	31.196	1.00	73.01
	ATOM	977	NE2	HIS	131	48.806	34.634	30.954	1.00	73.04
	ATOM	978	C	HIS	131	54.424	34.124	30.908	1.00	74.61
40	ATOM	979	O	HIS	131	54.419	33.049	31.514	1.00	74.70
	ATOM	980	N	GLN	132	55.374	34.502	30.046	1.00	76.14
	ATOM	981	CA	GLN	132	56.566	33.727	29.658	1.00	77.30
	ATOM	982	CB	GLN	132	56.536	32.293	30.218	1.00	77.68
	ATOM	983	CG	GLN	132	55.424	31.387	29.676	1.00	78.41
45	ATOM	984	CD	GLN	132	55.823	30.611	28.436	1.00	78.88
	ATOM	985	OE1	GLN	132	56.016	31.179	27.356	1.00	78.50
	ATOM	986	NE2	GLN	132	55.951	29.294	28.587	1.00	79.41
	ATOM	987	C	GLN	132	56.673	33.682	28.134	1.00	77.86
	ATOM	988	O	GLN	132	57.769	33.638	27.574	1.00	77.91
50	ATOM	989	N	MSE	133	55.520	33.703	27.472	1.00	78.39
	ATOM	990	CA	MSE	133	55.450	33.662	26.017	1.00	78.88
	ATOM	991	CB	MSE	133	53.989	33.684	25.551	1.00	80.96
	ATOM	992	CG	MSE	133	53.278	32.347	25.586	1.00	83.34
	ATOM	993	SE	MSE	133	51.991	32.273	26.846	1.00	87.09
55	ATOM	994	CE	MSE	133	52.168	30.521	27.421	1.00	84.33
	ATOM	995	C	MSE	133	56.174	34.812	25.333	1.00	77.90
	ATOM	996	O	MSE	133	55.552	35.548	24.567	1.00	78.34
	ATOM	997	N	LYS	134	57.470	34.973	25.587	1.00	75.97
	ATOM	998	CA	LYS	134	58.225	36.053	24.949	1.00	73.96

Figure 4 21/63

	ATOM	999	CB	LYS	134	58.976	36.879	25.997	1.00 73.14
	ATOM	1000	CG	LYS	134	59.676	38.125	25.454	1.00 72.28
	ATOM	1001	CD	LYS	134	58.697	39.250	25.141	1.00 70.99
	ATOM	1002	CE	LYS	134	59.415	40.586	24.935	1.00 70.06
5	ATOM	1003	NZ	LYS	134	60.234	40.640	23.687	1.00 69.46
	ATOM	1004	C	LYS	134	59.211	35.443	23.964	1.00 72.94
	ATOM	1005	O	LYS	134	59.727	36.123	23.077	1.00 72.63
	ATOM	1006	N	HIS	135	59.457	34.148	24.132	1.00 72.28
	ATOM	1007	CA	HIS	135	60.377	33.411	23.275	1.00 71.52
10	ATOM	1008	CB	HIS	135	61.359	32.584	24.119	1.00 71.15
	ATOM	1009	CG	HIS	135	60.719	31.448	24.859	1.00 70.88
	ATOM	1010	CD2	HIS	135	60.908	30.109	24.773	1.00 70.87
	ATOM	1011	ND1	HIS	135	59.750	31.635	25.822	1.00 70.81
	ATOM	1012	CE1	HIS	135	59.370	30.462	26.298	1.00 70.56
15	ATOM	1013	NE2	HIS	135	60.057	29.519	25.678	1.00 70.85
	ATOM	1014	C	HIS	135	59.584	32.482	22.365	1.00 71.26
	ATOM	1015	O	HIS	135	60.152	31.818	21.499	1.00 71.53
	ATOM	1016	N	LYS	136	58.272	32.434	22.574	1.00 70.85
	ATOM	1017	CA	LYS	136	57.393	31.590	21.766	1.00 70.33
20	ATOM	1018	CB	LYS	136	56.077	31.329	22.508	1.00 69.64
	ATOM	1019	CG	LYS	136	56.225	30.694	23.886	1.00 68.45
	ATOM	1020	CD	LYS	136	56.740	29.271	23.783	1.00 68.01
	ATOM	1021	CE	LYS	136	56.698	28.560	25.128	1.00 67.56
	ATOM	1022	NZ	LYS	136	55.303	28.356	25.623	1.00 66.87
25	ATOM	1023	C	LYS	136	57.088	32.296	20.443	1.00 70.46
	ATOM	1024	O	LYS	136	57.100	33.530	20.371	1.00 70.94
	ATOM	1025	N	LYS	137	56.828	31.519	19.396	1.00 70.16
	ATOM	1026	CA	LYS	137	56.505	32.096	18.096	1.00 69.80
	ATOM	1027	CB	LYS	137	57.505	31.642	17.023	1.00 71.09
30	ATOM	1028	CG	LYS	137	57.602	30.132	16.801	1.00 71.73
	ATOM	1029	CD	LYS	137	58.567	29.840	15.654	1.00 72.44
	ATOM	1030	CE	LYS	137	58.915	28.363	15.545	1.00 72.39
	ATOM	1031	NZ	LYS	137	59.919	28.136	14.463	1.00 72.59
	ATOM	1032	C	LYS	137	55.097	31.685	17.702	1.00 68.73
35	ATOM	1033	O	LYS	137	54.799	31.476	16.524	1.00 69.92
	ATOM	1034	N	LEU	138	54.243	31.579	18.716	1.00 66.57
	ATOM	1035	CA	LEU	138	52.841	31.193	18.586	1.00 63.82
	ATOM	1036	CB	LEU	138	52.057	31.788	19.748	1.00 63.11
	ATOM	1037	CG	LEU	138	52.364	31.145	21.092	1.00 62.89
40	ATOM	1038	CD1	LEU	138	51.924	32.068	22.220	1.00 62.68
	ATOM	1039	CD2	LEU	138	51.669	29.786	21.150	1.00 61.80
	ATOM	1040	C	LEU	138	52.114	31.553	17.294	1.00 62.26
	ATOM	1041	O	LEU	138	52.416	32.566	16.647	1.00 62.54
	ATOM	1042	N	PRO	139	51.149	30.708	16.894	1.00 60.11
45	ATOM	1043	CD	PRO	139	50.841	29.394	17.489	1.00 59.82
	ATOM	1044	CA	PRO	139	50.356	30.937	15.682	1.00 57.91
	ATOM	1045	CB	PRO	139	49.761	29.564	15.398	1.00 58.05
	ATOM	1046	CG	PRO	139	49.573	28.999	16.772	1.00 59.12
	ATOM	1047	C	PRO	139	49.302	31.968	16.101	1.00 55.89
50	ATOM	1048	O	PRO	139	48.469	31.693	16.973	1.00 55.71
	ATOM	1049	N	LEU	140	49.358	33.154	15.501	1.00 53.40
	ATOM	1050	CA	LEU	140	48.440	34.237	15.850	1.00 50.78
	ATOM	1051	CB	LEU	140	49.195	35.576	15.834	1.00 49.87
	ATOM	1052	CG	LEU	140	48.452	36.893	16.091	1.00 49.01
55	ATOM	1053	CD1	LEU	140	49.414	37.933	16.646	1.00 48.17
	ATOM	1054	CD2	LEU	140	47.825	37.389	14.801	1.00 48.88
	ATOM	1055	C	LEU	140	47.169	34.359	15.018	1.00 49.13
	ATOM	1056	O	LEU	140	47.211	34.368	13.785	1.00 49.12
	ATOM	1057	N	GLY	141	46.040	34.441	15.722	1.00 46.93

Figure 4

	ATOM	1058	CA	GLY	141	44.743	34.613	15.086	1.00	43.70
	ATOM	1059	C	GLY	141	44.324	36.041	15.402	1.00	41.11
	ATOM	1060	O	GLY	141	44.277	36.414	16.569	1.00	41.46
	ATOM	1061	N	PHE	142	44.018	36.842	14.388	1.00	38.27
5	ATOM	1062	CA	PHE	142	43.659	38.232	14.629	1.00	36.42
	ATOM	1063	CB	PHE	142	44.648	39.118	13.882	1.00	34.58
	ATOM	1064	CG	PHE	142	44.403	40.593	14.037	1.00	33.28
	ATOM	1065	CD1	PHE	142	43.941	41.124	15.229	1.00	32.86
	ATOM	1066	CD2	PHE	142	44.702	41.465	12.992	1.00	32.75
10	ATOM	1067	CE1	PHE	142	43.784	42.505	15.375	1.00	32.95
	ATOM	1068	CE2	PHE	142	44.551	42.845	13.125	1.00	31.57
	ATOM	1069	CZ	PHE	142	44.094	43.365	14.313	1.00	32.24
	ATOM	1070	C	PHE	142	42.224	38.652	14.300	1.00	36.83
	ATOM	1071	O	PHE	142	41.843	38.801	13.124	1.00	36.76
15	ATOM	1072	N	THR	143	41.423	38.848	15.347	1.00	35.96
	ATOM	1073	CA	THR	143	40.047	39.288	15.156	1.00	34.35
	ATOM	1074	CB	THR	143	39.179	38.997	16.373	1.00	33.98
	ATOM	1075	OG1	THR	143	38.947	37.586	16.472	1.00	33.45
	ATOM	1076	CG2	THR	143	37.854	39.750	16.255	1.00	33.35
20	ATOM	1077	C	THR	143	40.081	40.793	14.964	1.00	33.92
	ATOM	1078	O	THR	143	40.190	41.544	15.928	1.00	34.30
	ATOM	1079	N	PHE	144	40.009	41.227	13.716	1.00	33.00
	ATOM	1080	CA	PHE	144	40.029	42.649	13.383	1.00	31.69
	ATOM	1081	CB	PHE	144	40.891	42.842	12.132	1.00	29.18
25	ATOM	1082	CG	PHE	144	41.189	44.264	11.807	1.00	26.95
	ATOM	1083	CD1	PHE	144	41.727	45.108	12.763	1.00	26.21
	ATOM	1084	CD2	PHE	144	40.956	44.755	10.533	1.00	25.39
	ATOM	1085	CE1	PHE	144	42.026	46.428	12.450	1.00	26.79
	ATOM	1086	CE2	PHE	144	41.250	46.070	10.212	1.00	25.46
30	ATOM	1087	CZ	PHE	144	41.785	46.910	11.167	1.00	25.80
	ATOM	1088	C	PHE	144	38.562	42.981	13.112	1.00	32.02
	ATOM	1089	O	PHE	144	37.929	42.280	12.333	1.00	33.96
	ATOM	1090	N	SER	145	38.025	44.027	13.744	1.00	32.29
	ATOM	1091	CA	SER	145	36.602	44.387	13.600	1.00	31.56
35	ATOM	1092	CB	SER	145	35.993	44.689	14.968	1.00	31.79
	ATOM	1093	OG	SER	145	35.997	43.539	15.790	1.00	33.15
	ATOM	1094	C	SER	145	36.271	45.546	12.679	1.00	30.95
	ATOM	1095	O	SER	145	35.601	46.508	13.082	1.00	30.63
	ATOM	1096	N	PHE	146	36.723	45.456	11.439	1.00	30.27
40	ATOM	1097	CA	PHE	146	36.452	46.513	10.489	1.00	29.49
	ATOM	1098	CB	PHE	146	37.573	47.541	10.535	1.00	29.01
	ATOM	1099	CG	PHE	146	37.848	48.054	11.908	1.00	27.96
	ATOM	1100	CD1	PHE	146	38.654	47.336	12.775	1.00	28.87
	ATOM	1101	CD2	PHE	146	37.245	49.221	12.359	1.00	27.88
45	ATOM	1102	CE1	PHE	146	38.852	47.777	14.078	1.00	29.72
	ATOM	1103	CE2	PHE	146	37.434	49.670	13.659	1.00	26.92
	ATOM	1104	CZ	PHE	146	38.232	48.955	14.520	1.00	28.49
	ATOM	1105	C	PHE	146	36.318	45.937	9.093	1.00	29.49
	ATOM	1106	O	PHE	146	36.668	44.778	8.846	1.00	29.56
50	ATOM	1107	N	PRO	147	35.805	46.738	8.152	1.00	29.02
	ATOM	1108	CD	PRO	147	35.452	48.167	8.211	1.00	28.09
	ATOM	1109	CA	PRO	147	35.662	46.212	6.798	1.00	30.12
	ATOM	1110	CB	PRO	147	34.852	47.309	6.099	1.00	28.65
	ATOM	1111	CG	PRO	147	35.377	48.540	6.749	1.00	28.13
55	ATOM	1112	C	PRO	147	37.047	45.969	6.179	1.00	30.89
	ATOM	1113	O	PRO	147	37.938	46.821	6.263	1.00	32.17
	ATOM	1114	N	VAL	148	37.221	44.807	5.557	1.00	31.62
	ATOM	1115	CA	VAL	148	38.499	44.453	4.957	1.00	32.00
	ATOM	1116	CB	VAL	148	39.399	43.733	6.002	1.00	32.44

Figure 4 23/63

	ATOM	1117	CG1	VAL	148	40.471	42.940	5.311	1.00	33.36
	ATOM	1118	CG2	VAL	148	40.035	44.758	6.934	1.00	32.04
	ATOM	1119	C	VAL	148	38.351	43.557	3.733	1.00	31.54
	ATOM	1120	O	VAL	148	37.937	42.402	3.858	1.00	30.91
5	ATOM	1121	N	ALA	149	38.688	44.091	2.560	1.00	31.66
	ATOM	1122	CA	ALA	149	38.610	43.316	1.324	1.00	32.33
	ATOM	1123	CB	ALA	149	38.834	44.213	0.120	1.00	31.16
	ATOM	1124	C	ALA	149	39.723	42.288	1.428	1.00	33.43
	ATOM	1125	O	ALA	149	40.882	42.653	1.431	1.00	35.59
10	ATOM	1126	N	HIS	150	39.387	41.008	1.535	1.00	33.73
	ATOM	1127	CA	HIS	150	40.410	39.980	1.666	1.00	33.88
	ATOM	1128	CB	HIS	150	39.868	38.780	2.450	1.00	34.82
	ATOM	1129	CG	HIS	150	39.879	38.961	3.933	1.00	35.58
	ATOM	1130	CD2	HIS	150	40.344	38.162	4.921	1.00	36.49
15	ATOM	1131	ND1	HIS	150	39.329	40.061	4.555	1.00	36.45
	ATOM	1132	CE1	HIS	150	39.454	39.930	5.865	1.00	36.79
	ATOM	1133	NE2	HIS	150	40.067	38.786	6.114	1.00	36.38
	ATOM	1134	C	HIS	150	40.960	39.442	0.353	1.00	34.39
	ATOM	1135	O	HIS	150	40.245	39.364	-0.655	1.00	34.56
20	ATOM	1136	N	ALA	151	42.239	39.068	0.380	1.00	34.73
	ATOM	1137	CA	ALA	151	42.898	38.440	-0.762	1.00	34.53
	ATOM	1138	CB	ALA	151	44.334	38.949	-0.919	1.00	34.86
	ATOM	1139	C	ALA	151	42.894	36.968	-0.338	1.00	34.46
	ATOM	1140	O	ALA	151	42.734	36.065	-1.161	1.00	34.16
25	ATOM	1141	N	ASP	152	43.050	36.754	0.970	1.00	34.36
	ATOM	1142	CA	ASP	152	43.045	35.422	1.562	1.00	35.45
	ATOM	1143	CB	ASP	152	44.335	34.687	1.214	1.00	37.69
	ATOM	1144	CG	ASP	152	44.233	33.185	1.431	1.00	40.20
	ATOM	1145	OD1	ASP	152	43.219	32.717	2.007	1.00	40.73
30	ATOM	1146	OD2	ASP	152	45.177	32.464	1.018	1.00	42.29
	ATOM	1147	C	ASP	152	42.901	35.549	3.088	1.00	35.53
	ATOM	1148	O	ASP	152	43.048	36.642	3.642	1.00	35.08
	ATOM	1149	N	ILE	153	42.627	34.433	3.762	1.00	35.49
	ATOM	1150	CA	ILE	153	42.436	34.427	5.213	1.00	35.75
35	ATOM	1151	CB	ILE	153	42.258	32.984	5.754	1.00	35.32
	ATOM	1152	CG2	ILE	153	43.609	32.316	5.937	1.00	34.16
	ATOM	1153	CG1	ILE	153	41.593	33.022	7.130	1.00	35.44
	ATOM	1154	CD1	ILE	153	40.225	33.697	7.131	1.00	36.43
	ATOM	1155	C	ILE	153	43.571	35.079	6.011	1.00	36.77
40	ATOM	1156	O	ILE	153	43.450	35.278	7.229	1.00	36.40
	ATOM	1157	N	ASP	154	44.665	35.411	5.332	1.00	37.10
	ATOM	1158	CA	ASP	154	45.815	36.003	6.000	1.00	37.27
	ATOM	1159	CB	ASP	154	46.982	35.013	5.991	1.00	38.98
	ATOM	1160	CG	ASP	154	47.795	35.079	4.703	1.00	41.58
45	ATOM	1161	OD1	ASP	154	47.215	34.890	3.605	1.00	42.46
	ATOM	1162	OD2	ASP	154	49.022	35.331	4.789	1.00	42.65
	ATOM	1163	C	ASP	154	46.233	37.287	5.307	1.00	36.74
	ATOM	1164	O	ASP	154	47.360	37.751	5.471	1.00	37.07
	ATOM	1165	N	ALA	155	45.328	37.865	4.531	1.00	35.91
50	ATOM	1166	CA	ALA	155	45.650	39.093	3.830	1.00	36.20
	ATOM	1167	CB	ALA	155	46.522	38.771	2.621	1.00	36.22
	ATOM	1168	C	ALA	155	44.412	39.864	3.387	1.00	36.20
	ATOM	1169	O	ALA	155	43.490	39.289	2.820	1.00	36.87
	ATOM	1170	N	GLY	156	44.402	41.168	3.642	1.00	36.26
55	ATOM	1171	CA	GLY	156	43.279	41.997	3.245	1.00	37.08
	ATOM	1172	C	GLY	156	43.481	43.446	3.647	1.00	38.10
	ATOM	1173	O	GLY	156	44.027	43.727	4.711	1.00	38.52
	ATOM	1174	N	ILE	157	43.052	44.377	2.805	1.00	39.16
	ATOM	1175	CA	ILE	157	43.203	45.789	3.125	1.00	41.42

Figure 4 24/63

	ATOM	1176	CB	ILE	157	43.389	46.646	1.842	1.00	42.84
	ATOM	1177	CG2	ILE	157	44.844	46.550	1.349	1.00	44.32
	ATOM	1178	CG1	ILE	157	42.399	46.193	0.761	1.00	43.93
	ATOM	1179	CD1	ILE	157	42.630	46.838	-0.615	1.00	44.55
5	ATOM	1180	C	ILE	157	42.010	46.331	3.921	1.00	42.26
	ATOM	1181	O	ILE	157	40.864	45.912	3.732	1.00	42.28
	ATOM	1182	N	LEU	158	42.300	47.259	4.824	1.00	42.54
	ATOM	1183	CA	LEU	158	41.283	47.873	5.648	1.00	43.22
	ATOM	1184	CB	LEU	158	41.928	48.504	6.884	1.00	44.12
10	ATOM	1185	CG	LEU	158	41.090	49.514	7.670	1.00	44.84
	ATOM	1186	CD1	LEU	158	40.020	48.782	8.472	1.00	45.23
	ATOM	1187	CD2	LEU	158	42.006	50.320	8.590	1.00	45.09
	ATOM	1188	C	LEU	158	40.548	48.947	4.855	1.00	43.56
	ATOM	1189	O	LEU	158	40.984	50.099	4.801	1.00	43.77
15	ATOM	1190	N	LEU	159	39.434	48.569	4.239	1.00	43.40
	ATOM	1191	CA	LEU	159	38.634	49.508	3.465	1.00	43.01
	ATOM	1192	CB	LEU	159	37.238	48.935	3.280	1.00	43.36
	ATOM	1193	CG	LEU	159	37.279	47.599	2.539	1.00	43.44
	ATOM	1194	CD1	LEU	159	36.020	46.808	2.829	1.00	44.00
20	ATOM	1195	CD2	LEU	159	37.443	47.857	1.050	1.00	42.93
	ATOM	1196	C	LEU	159	38.564	50.879	4.139	1.00	42.62
	ATOM	1197	O	LEU	159	38.745	51.905	3.488	1.00	43.03
	ATOM	1198	N	ASN	160	38.297	50.902	5.440	1.00	42.20
	ATOM	1199	CA	ASN	160	38.243	52.169	6.170	1.00	41.99
25	ATOM	1200	CB	ASN	160	37.347	53.197	5.447	1.00	42.23
	ATOM	1201	CG	ASN	160	35.913	52.733	5.295	1.00	43.38
	ATOM	1202	OD1	ASN	160	35.225	53.102	4.334	1.00	42.38
	ATOM	1203	ND2	ASN	160	35.444	51.934	6.250	1.00	44.48
	ATOM	1204	C	ASN	160	37.813	51.988	7.616	1.00	41.13
30	ATOM	1205	O	ASN	160	37.359	50.913	8.011	1.00	41.17
	ATOM	1206	N	TRP	161	37.980	53.043	8.403	1.00	40.24
	ATOM	1207	CA	TRP	161	37.652	53.004	9.824	1.00	39.69
	ATOM	1208	CB	TRP	161	38.522	54.003	10.602	1.00	39.33
	ATOM	1209	CG	TRP	161	39.987	53.640	10.769	1.00	39.07
35	ATOM	1210	CD2	TRP	161	40.527	52.469	11.411	1.00	38.63
	ATOM	1211	CE2	TRP	161	41.931	52.616	11.438	1.00	38.27
	ATOM	1212	CE3	TRP	161	39.960	51.317	11.972	1.00	38.43
	ATOM	1213	CD1	TRP	161	41.060	54.417	10.436	1.00	38.40
	ATOM	1214	NE1	TRP	161	42.228	53.812	10.840	1.00	38.42
40	ATOM	1215	CZ2	TRP	161	42.778	51.659	12.000	1.00	38.26
	ATOM	1216	CZ3	TRP	161	40.809	50.357	12.538	1.00	38.07
	ATOM	1217	CH2	TRP	161	42.200	50.540	12.545	1.00	38.37
	ATOM	1218	C	TRP	161	36.196	53.301	10.150	1.00	39.07
	ATOM	1219	O	TRP	161	35.578	54.193	9.562	1.00	39.38
45	ATOM	1220	N	THR	162	35.668	52.555	11.114	1.00	38.45
	ATOM	1221	CA	THR	162	34.302	52.734	11.593	1.00	38.37
	ATOM	1222	CB	THR	162	33.381	51.600	11.125	1.00	37.71
	ATOM	1223	OG1	THR	162	33.926	50.338	11.548	1.00	37.02
	ATOM	1224	CG2	THR	162	33.226	51.635	9.617	1.00	36.52
50	ATOM	1225	C	THR	162	34.357	52.702	13.121	1.00	38.24
	ATOM	1226	O	THR	162	35.405	52.443	13.703	1.00	37.86
	ATOM	1227	N	LYS	163	33.231	52.968	13.770	1.00	38.99
	ATOM	1228	CA	LYS	163	33.192	52.941	15.222	1.00	39.72
	ATOM	1229	CB	LYS	163	33.510	51.528	15.728	1.00	38.16
55	ATOM	1230	CG	LYS	163	32.467	50.487	15.311	1.00	36.62
	ATOM	1231	CD	LYS	163	32.727	49.108	15.918	1.00	34.66
	ATOM	1232	CE	LYS	163	33.829	48.349	15.195	1.00	33.22
	ATOM	1233	NZ	LYS	163	34.068	47.031	15.850	1.00	32.19
	ATOM	1234	C	LYS	163	34.142	53.956	15.848	1.00	40.71

Figure 4 25/63

	ATOM	1235	O	LYS	163	34.690	53.723	16.931	1.00	40.69
	ATOM	1236	N	GLY	164	34.338	55.076	15.156	1.00	41.81
	ATOM	1237	CA	GLY	164	35.187	56.139	15.672	1.00	43.90
	ATOM	1238	C	GLY	164	36.685	56.031	15.463	1.00	45.41
5	ATOM	1239	O	GLY	164	37.375	57.055	15.381	1.00	45.25
	ATOM	1240	N	PHE	165	37.190	54.802	15.397	1.00	47.06
	ATOM	1241	CA	PHE	165	38.613	54.560	15.197	1.00	48.70
	ATOM	1242	CB	PHE	165	38.852	53.117	14.767	1.00	47.20
	ATOM	1243	CG	PHE	165	39.290	52.222	15.870	1.00	45.64
10	ATOM	1244	CD1	PHE	165	38.443	51.937	16.929	1.00	45.87
	ATOM	1245	CD2	PHE	165	40.544	51.632	15.833	1.00	45.19
	ATOM	1246	CE1	PHE	165	38.840	51.064	17.945	1.00	46.28
	ATOM	1247	CE2	PHE	165	40.952	50.763	16.834	1.00	45.80
	ATOM	1248	CZ	PHE	165	40.098	50.475	17.896	1.00	45.96
15	ATOM	1249	C	PHE	165	39.250	55.471	14.154	1.00	50.94
	ATOM	1250	O	PHE	165	38.633	55.823	13.143	1.00	50.36
	ATOM	1251	N	LYS	166	40.500	55.838	14.415	1.00	53.77
	ATOM	1252	CA	LYS	166	41.275	56.680	13.514	1.00	56.56
	ATOM	1253	CB	LYS	166	41.050	58.170	13.822	1.00	56.16
20	ATOM	1254	CG	LYS	166	39.720	58.697	13.290	1.00	56.44
	ATOM	1255	CD	LYS	166	39.524	58.320	11.812	1.00	56.54
	ATOM	1256	CE	LYS	166	38.131	58.694	11.305	1.00	56.74
	ATOM	1257	NZ	LYS	166	37.863	58.198	9.922	1.00	56.86
	ATOM	1258	C	LYS	166	42.751	56.322	13.640	1.00	58.33
25	ATOM	1259	O	LYS	166	43.180	55.747	14.651	1.00	58.69
	ATOM	1260	N	ALA	167	43.510	56.647	12.597	1.00	59.76
	ATOM	1261	CA	ALA	167	44.943	56.375	12.543	1.00	61.43
	ATOM	1262	CB	ALA	167	45.220	54.901	12.834	1.00	60.92
	ATOM	1263	C	ALA	167	45.401	56.725	11.137	1.00	62.76
30	ATOM	1264	O	ALA	167	45.147	55.967	10.197	1.00	63.38
	ATOM	1265	N	SER	168	46.066	57.872	10.999	1.00	63.98
	ATOM	1266	CA	SER	168	46.556	58.345	9.704	1.00	64.43
	ATOM	1267	CB	SER	168	47.636	59.414	9.903	1.00	64.96
	ATOM	1268	OG	SER	168	47.130	60.546	10.594	1.00	65.76
35	ATOM	1269	C	SER	168	47.115	57.216	8.846	1.00	64.59
	ATOM	1270	O	SER	168	47.805	56.322	9.347	1.00	64.35
	ATOM	1271	N	GLY	169	46.800	57.260	7.553	1.00	64.75
	ATOM	1272	CA	GLY	169	47.280	56.245	6.632	1.00	65.55
	ATOM	1273	C	GLY	169	47.158	54.821	7.142	1.00	65.88
40	ATOM	1274	O	GLY	169	48.151	54.097	7.255	1.00	65.72
	ATOM	1275	N	ALA	170	45.936	54.416	7.465	1.00	66.32
	ATOM	1276	CA	ALA	170	45.699	53.065	7.947	1.00	66.82
	ATOM	1277	CB	ALA	170	44.930	53.100	9.256	1.00	66.65
	ATOM	1278	C	ALA	170	44.890	52.346	6.879	1.00	67.02
45	ATOM	1279	O	ALA	170	45.209	51.226	6.477	1.00	67.31
	ATOM	1280	N	GLU	171	43.847	53.017	6.410	1.00	66.85
	ATOM	1281	CA	GLU	171	42.979	52.463	5.387	1.00	66.80
	ATOM	1282	CB	GLU	171	41.705	53.292	5.287	1.00	67.90
	ATOM	1283	CG	GLU	171	41.958	54.783	5.279	1.00	69.27
50	ATOM	1284	CD	GLU	171	40.850	55.552	4.590	1.00	70.17
	ATOM	1285	OE1	GLU	171	40.789	55.506	3.340	1.00	70.45
	ATOM	1286	OE2	GLU	171	40.038	56.191	5.296	1.00	70.67
	ATOM	1287	C	GLU	171	43.666	52.427	4.032	1.00	65.92
	ATOM	1288	O	GLU	171	44.469	53.301	3.711	1.00	66.22
55	ATOM	1289	N	GLY	172	43.339	51.408	3.242	1.00	64.69
	ATOM	1290	CA	GLY	172	43.922	51.265	1.925	1.00	62.79
	ATOM	1291	C	GLY	172	45.096	50.312	1.882	1.00	61.61
	ATOM	1292	O	GLY	172	45.493	49.884	0.805	1.00	61.59
	ATOM	1293	N	ASN	173	45.643	49.965	3.045	1.00	60.93

Figure 4   26/63

	ATOM	1294	CA	ASN	173	46.800	49.065	3.115	1.00	60.42
	ATOM	1295	CB	ASN	173	47.922	49.722	3.913	1.00	61.72
	ATOM	1296	CG	ASN	173	48.035	51.201	3.631	1.00	62.78
	ATOM	1297	OD1	ASN	173	48.367	51.605	2.515	1.00	63.29
5	ATOM	1298	ND2	ASN	173	47.741	52.024	4.637	1.00	63.06
	ATOM	1299	C	ASN	173	46.463	47.747	3.771	1.00	59.26
	ATOM	1300	O	ASN	173	45.440	47.624	4.430	1.00	59.57
	ATOM	1301	N	ASN	174	47.336	46.763	3.598	1.00	58.79
	ATOM	1302	CA	ASN	174	47.126	45.447	4.196	1.00	58.46
10	ATOM	1303	CB	ASN	174	48.264	44.495	3.793	1.00	57.45
	ATOM	1304	CG	ASN	174	48.104	43.093	4.375	1.00	57.22
	ATOM	1305	OD1	ASN	174	48.757	42.144	3.924	1.00	56.21
	ATOM	1306	ND2	ASN	174	47.245	42.957	5.382	1.00	56.76
	ATOM	1307	C	ASN	174	47.083	45.615	5.712	1.00	58.42
15	ATOM	1308	O	ASN	174	47.927	46.302	6.281	1.00	59.03
	ATOM	1309	N	VAL	175	46.091	45.008	6.359	1.00	58.23
	ATOM	1310	CA	VAL	175	45.966	45.106	7.809	1.00	57.79
	ATOM	1311	CB	VAL	175	44.544	44.765	8.295	1.00	57.69
	ATOM	1312	CG1	VAL	175	44.461	44.933	9.807	1.00	56.81
20	ATOM	1313	CG2	VAL	175	43.531	45.665	7.603	1.00	57.69
	ATOM	1314	C	VAL	175	46.944	44.150	8.470	1.00	57.62
	ATOM	1315	O	VAL	175	47.734	44.560	9.319	1.00	57.89
	ATOM	1316	N	VAL	176	46.896	42.878	8.086	1.00	57.24
	ATOM	1317	CA	VAL	176	47.818	41.904	8.660	1.00	57.25
25	ATOM	1318	CB	VAL	176	47.638	40.501	8.037	1.00	57.27
	ATOM	1319	CG1	VAL	176	48.597	39.511	8.701	1.00	56.21
	ATOM	1320	CG2	VAL	176	46.196	40.035	8.199	1.00	56.28
	ATOM	1321	C	VAL	176	49.232	42.396	8.362	1.00	57.38
	ATOM	1322	O	VAL	176	50.212	41.911	8.926	1.00	57.30
30	ATOM	1323	N	GLY	177	49.319	43.374	7.467	1.00	57.41
	ATOM	1324	CA	GLY	177	50.605	43.939	7.103	1.00	57.60
	ATOM	1325	C	GLY	177	51.135	44.878	8.170	1.00	57.50
	ATOM	1326	O	GLY	177	52.171	44.605	8.781	1.00	58.09
	ATOM	1327	N	LEU	178	50.425	45.982	8.396	1.00	56.68
35	ATOM	1328	CA	LEU	178	50.837	46.959	9.396	1.00	55.42
	ATOM	1329	CB	LEU	178	49.710	47.968	9.646	1.00	55.02
	ATOM	1330	CG	LEU	178	49.394	48.906	8.466	1.00	54.15
	ATOM	1331	CD1	LEU	178	48.158	49.743	8.766	1.00	53.80
	ATOM	1332	CD2	LEU	178	50.588	49.815	8.197	1.00	54.17
40	ATOM	1333	C	LEU	178	51.247	46.279	10.701	1.00	54.84
	ATOM	1334	O	LEU	178	52.177	46.717	11.375	1.00	55.07
	ATOM	1335	N	LEU	179	50.575	45.192	11.050	1.00	53.85
	ATOM	1336	CA	LEU	179	50.917	44.491	12.274	1.00	53.57
	ATOM	1337	CB	LEU	179	49.882	43.409	12.582	1.00	52.75
45	ATOM	1338	CG	LEU	179	50.099	42.671	13.907	1.00	52.23
	ATOM	1339	CD1	LEU	179	49.689	43.580	15.056	1.00	51.63
	ATOM	1340	CD2	LEU	179	49.286	41.381	13.935	1.00	51.34
	ATOM	1341	C	LEU	179	52.286	43.845	12.128	1.00	54.26
	ATOM	1342	O	LEU	179	53.070	43.796	13.075	1.00	54.60
50	ATOM	1343	N	ARG	180	52.576	43.343	10.932	1.00	54.59
	ATOM	1344	CA	ARG	180	53.855	42.679	10.688	1.00	54.08
	ATOM	1345	CB	ARG	180	53.824	41.911	9.357	1.00	52.59
	ATOM	1346	CG	ARG	180	53.273	40.498	9.515	1.00	50.37
	ATOM	1347	CD	ARG	180	53.276	39.702	8.223	1.00	47.24
55	ATOM	1348	NE	ARG	180	52.610	38.420	8.425	1.00	45.06
	ATOM	1349	CZ	ARG	180	51.979	37.754	7.462	1.00	43.97
	ATOM	1350	NH1	ARG	180	51.935	38.256	6.226	1.00	42.53
	ATOM	1351	NH2	ARG	180	51.366	36.601	7.735	1.00	42.95
	ATOM	1352	C	ARG	180	55.059	43.605	10.732	1.00	54.76

Figure 4 27/63

	ATOM	1353	O	ARG	180	56.009	43.343	11.473	1.00 54.65
	ATOM	1354	N	ASP	181	55.036	44.681	9.951	1.00 55.34
	ATOM	1355	CA	ASP	181	56.169	45.593	9.972	1.00 56.60
	ATOM	1356	CB	ASP	181	56.266	46.386	8.649	1.00 56.43
5	ATOM	1357	CG	ASP	181	55.132	47.382	8.448	1.00 55.64
	ATOM	1358	OD1	ASP	181	54.658	47.483	7.294	1.00 55.20
	ATOM	1359	OD2	ASP	181	54.734	48.076	9.416	1.00 55.23
	ATOM	1360	C	ASP	181	56.115	46.514	11.199	1.00 57.64
	ATOM	1361	O	ASP	181	56.510	47.685	11.153	1.00 57.96
10	ATOM	1362	N	ALA	182	55.634	45.947	12.303	1.00 57.87
	ATOM	1363	CA	ALA	182	55.524	46.646	13.577	1.00 57.84
	ATOM	1364	CB	ALA	182	54.078	47.048	13.836	1.00 58.19
	ATOM	1365	C	ALA	182	56.013	45.683	14.657	1.00 57.83
	ATOM	1366	O	ALA	182	56.681	46.094	15.611	1.00 58.32
15	ATOM	1367	N	ILE	183	55.669	44.404	14.505	1.00 57.35
	ATOM	1368	CA	ILE	183	56.109	43.381	15.448	1.00 57.40
	ATOM	1369	CB	ILE	183	55.374	42.036	15.233	1.00 56.09
	ATOM	1370	CG2	ILE	183	56.025	40.932	16.074	1.00 55.25
	ATOM	1371	CG1	ILE	183	53.904	42.174	15.628	1.00 55.30
20	ATOM	1372	CD1	ILE	183	53.115	40.881	15.505	1.00 54.14
	ATOM	1373	C	ILE	183	57.600	43.164	15.199	1.00 58.51
	ATOM	1374	O	ILE	183	58.294	42.531	16.002	1.00 59.24
	ATOM	1375	N	LYS	184	58.093	43.689	14.077	1.00 59.04
	ATOM	1376	CA	LYS	184	59.508	43.550	13.757	1.00 59.19
25	ATOM	1377	CB	LYS	184	59.719	43.243	12.268	1.00 59.15
	ATOM	1378	CG	LYS	184	59.356	44.354	11.310	1.00 58.36
	ATOM	1379	CD	LYS	184	59.566	43.897	9.868	1.00 58.59
	ATOM	1380	CE	LYS	184	58.637	42.735	9.500	1.00 59.26
	ATOM	1381	NZ	LYS	184	58.751	42.306	8.067	1.00 59.63
30	ATOM	1382	C	LYS	184	60.270	44.806	14.155	1.00 59.27
	ATOM	1383	O	LYS	184	61.382	44.705	14.667	1.00 59.28
	ATOM	1384	N	ARG	185	59.695	45.984	13.923	1.00 59.21
	ATOM	1385	CA	ARG	185	60.383	47.211	14.331	1.00 59.69
	ATOM	1386	CB	ARG	185	59.545	48.458	14.060	1.00 59.70
35	ATOM	1387	CG	ARG	185	59.278	48.772	12.610	1.00 60.85
	ATOM	1388	CD	ARG	185	59.138	50.280	12.443	1.00 60.89
	ATOM	1389	NE	ARG	185	58.121	50.628	11.459	1.00 62.26
	ATOM	1390	CZ	ARG	185	56.819	50.403	11.620	1.00 61.84
	ATOM	1391	NH1	ARG	185	56.372	49.828	12.731	1.00 61.22
40	ATOM	1392	NH2	ARG	185	55.966	50.754	10.666	1.00 62.23
	ATOM	1393	C	ARG	185	60.574	47.104	15.836	1.00 60.41
	ATOM	1394	O	ARG	185	61.630	47.430	16.384	1.00 60.45
	ATOM	1395	N	ARG	186	59.518	46.633	16.489	1.00 61.07
	ATOM	1396	CA	ARG	186	59.489	46.460	17.933	1.00 61.42
45	ATOM	1397	CB	ARG	186	58.066	46.055	18.358	1.00 61.16
	ATOM	1398	CG	ARG	186	57.666	46.433	19.786	1.00 61.08
	ATOM	1399	CD	ARG	186	58.249	45.473	20.828	1.00 60.87
	ATOM	1400	NE	ARG	186	57.917	45.894	22.188	1.00 61.44
	ATOM	1401	CZ	ARG	186	58.294	45.246	23.288	1.00 60.67
50	ATOM	1402	NH1	ARG	186	59.024	44.133	23.201	1.00 60.28
	ATOM	1403	NH2	ARG	186	57.942	45.712	24.481	1.00 61.46
	ATOM	1404	C	ARG	186	60.516	45.399	18.344	1.00 61.85
	ATOM	1405	O	ARG	186	60.980	44.610	17.514	1.00 62.16
	ATOM	1406	N	GLY	187	60.873	45.401	19.628	1.00 62.07
55	ATOM	1407	CA	GLY	187	61.843	44.455	20.157	1.00 62.22
	ATOM	1408	C	GLY	187	61.591	43.017	19.754	1.00 62.50
	ATOM	1409	O	GLY	187	60.541	42.692	19.202	1.00 62.37
	ATOM	1410	N	ASP	188	62.556	42.148	20.036	1.00 63.08
	ATOM	1411	CA	ASP	188	62.414	40.746	19.684	1.00 62.67

Figure 4   28/63

	ATOM	1412	CB	ASP	188	63.465	39.873	20.373	1.00	61.80
	ATOM	1413	CG	ASP	188	63.027	38.409	20.468	1.00	60.64
	ATOM	1414	OD1	ASP	188	62.125	38.107	21.289	1.00	60.77
	ATOM	1415	OD2	ASP	188	63.565	37.563	19.715	1.00	60.43
5	ATOM	1416	C	ASP	188	61.047	40.193	20.022	1.00	63.58
	ATOM	1417	O	ASP	188	60.441	40.539	21.044	1.00	62.69
	ATOM	1418	N	PHE	189	60.599	39.309	19.138	1.00	64.49
	ATOM	1419	CA	PHE	189	59.327	38.632	19.249	1.00	64.75
	ATOM	1420	CB	PHE	189	58.233	39.629	19.598	1.00	64.84
10	ATOM	1421	CG	PHE	189	56.886	39.010	19.689	1.00	65.46
	ATOM	1422	CD1	PHE	189	56.707	37.824	20.402	1.00	65.54
	ATOM	1423	CD2	PHE	189	55.795	39.592	19.052	1.00	65.28
	ATOM	1424	CE1	PHE	189	55.455	37.224	20.481	1.00	65.61
	ATOM	1425	CE2	PHE	189	54.542	39.007	19.122	1.00	65.71
15	ATOM	1426	CZ	PHE	189	54.369	37.819	19.839	1.00	65.57
	ATOM	1427	C	PHE	189	59.018	37.952	17.919	1.00	65.33
	ATOM	1428	O	PHE	189	58.921	38.609	16.881	1.00	64.91
	ATOM	1429	N	GLU	190	58.879	36.631	17.956	1.00	66.13
	ATOM	1430	CA	GLU	190	58.584	35.854	16.752	1.00	66.57
20	ATOM	1431	CB	GLU	190	59.387	34.545	16.755	1.00	66.34
	ATOM	1432	CG	GLU	190	60.778	34.649	17.389	1.00	64.66
	ATOM	1433	CD	GLU	190	61.908	34.356	16.411	1.00	64.02
	ATOM	1434	OE1	GLU	190	63.054	34.161	16.874	1.00	63.09
	ATOM	1435	OE2	GLU	190	61.658	34.327	15.186	1.00	63.04
25	ATOM	1436	C	GLU	190	57.093	35.528	16.745	1.00	67.09
	ATOM	1437	O	GLU	190	56.609	34.828	17.638	1.00	67.36
	ATOM	1438	N	MSE	191	56.367	36.030	15.747	1.00	67.05
	ATOM	1439	CA	MSE	191	54.928	35.775	15.666	1.00	66.65
	ATOM	1440	CB	MSE	191	54.164	36.920	16.347	1.00	69.47
30	ATOM	1441	CG	MSE	191	52.867	36.492	17.037	1.00	72.30
	ATOM	1442	SE	MSE	191	53.120	35.293	18.409	1.00	78.56
	ATOM	1443	CE	MSE	191	51.941	35.893	19.581	1.00	75.88
	ATOM	1444	C	MSE	191	54.412	35.590	14.230	1.00	64.85
	ATOM	1445	O	MSE	191	54.399	36.538	13.435	1.00	64.30
35	ATOM	1446	N	ASP	192	53.977	34.368	13.910	1.00	62.82
	ATOM	1447	CA	ASP	192	53.449	34.051	12.580	1.00	60.76
	ATOM	1448	CB	ASP	192	53.774	32.607	12.207	1.00	61.24
	ATOM	1449	CG	ASP	192	55.210	32.427	11.792	1.00	61.76
	ATOM	1450	OD1	ASP	192	55.684	33.219	10.947	1.00	62.45
40	ATOM	1451	OD2	ASP	192	55.863	31.492	12.299	1.00	62.32
	ATOM	1452	C	ASP	192	51.942	34.266	12.459	1.00	59.03
	ATOM	1453	O	ASP	192	51.143	33.375	12.767	1.00	58.37
	ATOM	1454	N	VAL	193	51.567	35.453	11.991	1.00	57.00
	ATOM	1455	CA	VAL	193	50.167	35.818	11.818	1.00	54.85
45	ATOM	1456	CB	VAL	193	50.034	37.305	11.454	1.00	55.09
	ATOM	1457	CG1	VAL	193	48.568	37.712	11.448	1.00	54.84
	ATOM	1458	CG2	VAL	193	50.826	38.146	12.441	1.00	54.87
	ATOM	1459	C	VAL	193	49.473	34.977	10.746	1.00	53.19
	ATOM	1460	O	VAL	193	49.500	35.303	9.555	1.00	52.03
50	ATOM	1461	N	VAL	194	48.854	33.894	11.205	1.00	51.82
	ATOM	1462	CA	VAL	194	48.126	32.949	10.367	1.00	50.66
	ATOM	1463	CB	VAL	194	47.841	31.644	11.174	1.00	51.08
	ATOM	1464	CG1	VAL	194	46.686	30.860	10.554	1.00	52.09
	ATOM	1465	CG2	VAL	194	49.091	30.778	11.211	1.00	51.33
55	ATOM	1466	C	VAL	194	46.798	33.498	9.808	1.00	49.99
	ATOM	1467	O	VAL	194	46.677	33.726	8.602	1.00	49.40
	ATOM	1468	N	ALA	195	45.813	33.723	10.683	1.00	48.93
	ATOM	1469	CA	ALA	195	44.499	34.193	10.251	1.00	47.60
	ATOM	1470	CB	ALA	195	43.467	33.123	10.572	1.00	47.58

Figure 4

	ATOM	1471	C	ALA	195	43.992	35.546	10.760	1.00 46.68
	ATOM	1472	O	ALA	195	44.344	35.996	11.851	1.00 46.16
	ATOM	1473	N	MSE	196	43.157	36.182	9.940	1.00 45.43
	ATOM	1474	CA	MSE	196	42.521	37.459	10.279	1.00 44.60
5	ATOM	1475	CB	MSE	196	43.079	38.623	9.451	1.00 45.32
	ATOM	1476	CG	MSE	196	42.329	39.925	9.716	1.00 47.29
	ATOM	1477	SE	MSE	196	42.937	41.426	8.852	1.00 53.21
	ATOM	1478	CE	MSE	196	44.264	41.920	9.982	1.00 51.44
	ATOM	1479	C	MSE	196	41.019	37.333	10.002	1.00 43.09
10	ATOM	1480	O	MSE	196	40.610	36.973	8.892	1.00 43.71
	ATOM	1481	N	VAL	197	40.190	37.631	10.996	1.00 40.47
	ATOM	1482	CA	VAL	197	38.751	37.514	10.799	1.00 37.00
	ATOM	1483	CB	VAL	197	38.240	36.228	11.458	1.00 37.31
	ATOM	1484	CG1	VAL	197	38.840	35.004	10.766	1.00 36.64
15	ATOM	1485	CG2	VAL	197	38.643	36.217	12.914	1.00 36.88
	ATOM	1486	C	VAL	197	37.991	38.710	11.354	1.00 35.22
	ATOM	1487	O	VAL	197	38.561	39.544	12.057	1.00 35.21
	ATOM	1488	N	ASN	198	36.708	38.801	11.015	1.00 33.39
	ATOM	1489	CA	ASN	198	35.830	39.883	11.491	1.00 30.23
20	ATOM	1490	CB	ASN	198	34.740	40.175	10.446	1.00 30.65
	ATOM	1491	CG	ASN	198	33.801	41.309	10.852	1.00 31.35
	ATOM	1492	OD1	ASN	198	32.907	41.128	11.686	1.00 32.70
	ATOM	1493	ND2	ASN	198	33.997	42.486	10.251	1.00 30.53
	ATOM	1494	C	ASN	198	35.217	39.356	12.780	1.00 28.41
25	ATOM	1495	O	ASN	198	35.052	38.143	12.937	1.00 26.14
	ATOM	1496	N	ASP	199	34.892	40.252	13.711	1.00 27.77
	ATOM	1497	CA	ASP	199	34.325	39.816	14.990	1.00 26.87
	ATOM	1498	CB	ASP	199	34.156	41.007	15.945	1.00 26.75
	ATOM	1499	CG	ASP	199	33.254	42.097	15.396	1.00 26.24
30	ATOM	1500	OD1	ASP	199	33.221	42.292	14.167	1.00 26.90
	ATOM	1501	OD2	ASP	199	32.587	42.777	16.205	1.00 26.19
	ATOM	1502	C	ASP	199	33.027	39.034	14.843	1.00 26.43
	ATOM	1503	O	ASP	199	32.715	38.188	15.684	1.00 27.02
	ATOM	1504	N	THR	200	32.291	39.292	13.763	1.00 25.45
35	ATOM	1505	CA	THR	200	31.050	38.585	13.510	1.00 25.65
	ATOM	1506	CB	THR	200	30.261	39.193	12.339	1.00 25.75
	ATOM	1507	OG1	THR	200	31.008	39.044	11.130	1.00 26.04
	ATOM	1508	CG2	THR	200	30.002	40.672	12.573	1.00 26.48
	ATOM	1509	C	THR	200	31.383	37.155	13.143	1.00 26.96
40	ATOM	1510	O	THR	200	30.832	36.211	13.712	1.00 27.62
	ATOM	1511	N	VAL	201	32.295	36.990	12.189	1.00 28.07
	ATOM	1512	CA	VAL	201	32.695	35.654	11.742	1.00 28.50
	ATOM	1513	CB	VAL	201	33.785	35.726	10.665	1.00 29.26
	ATOM	1514	CG1	VAL	201	34.056	34.332	10.123	1.00 31.22
45	ATOM	1515	CG2	VAL	201	33.370	36.684	9.546	1.00 27.90
	ATOM	1516	C	VAL	201	33.231	34.818	12.901	1.00 29.16
	ATOM	1517	O	VAL	201	32.816	33.676	13.101	1.00 29.44
	ATOM	1518	N	ALA	202	34.156	35.395	13.663	1.00 30.31
	ATOM	1519	CA	ALA	202	34.752	34.710	14.812	1.00 32.23
50	ATOM	1520	CB	ALA	202	35.591	35.705	15.643	1.00 31.72
	ATOM	1521	C	ALA	202	33.688	34.070	15.696	1.00 33.37
	ATOM	1522	O	ALA	202	33.789	32.894	16.073	1.00 34.14
	ATOM	1523	N	THR	203	32.667	34.858	16.019	1.00 34.41
	ATOM	1524	CA	THR	203	31.566	34.422	16.870	1.00 35.37
55	ATOM	1525	CB	THR	203	30.614	35.604	17.117	1.00 36.27
	ATOM	1526	OG1	THR	203	31.370	36.708	17.645	1.00 37.04
	ATOM	1527	CG2	THR	203	29.500	35.213	18.090	1.00 35.19
	ATOM	1528	C	THR	203	30.800	33.260	16.242	1.00 36.08
	ATOM	1529	O	THR	203	30.538	32.241	16.891	1.00 35.34

Figure 4

	ATOM	1530	N	MSE	204	30.433	33.415	14.978	1.00	36.89
	ATOM	1531	CA	MSE	204	29.722	32.348	14.299	1.00	37.94
	ATOM	1532	CB	MSE	204	29.582	32.665	12.811	1.00	39.76
	ATOM	1533	CG	MSE	204	29.065	31.504	11.954	1.00	40.74
5	ATOM	1534	SE	MSE	204	29.135	31.967	10.181	1.00	45.75
	ATOM	1535	CE	MSE	204	30.643	31.057	9.627	1.00	45.26
	ATOM	1536	C	MSE	204	30.531	31.075	14.465	1.00	38.36
	ATOM	1537	O	MSE	204	30.024	30.064	14.954	1.00	37.86
	ATOM	1538	N	ILE	205	31.798	31.148	14.061	1.00	38.79
10	ATOM	1539	CA	ILE	205	32.696	30.008	14.137	1.00	40.09
	ATOM	1540	CB	ILE	205	34.178	30.451	13.981	1.00	39.81
	ATOM	1541	CG2	ILE	205	35.098	29.240	14.072	1.00	39.47
	ATOM	1542	CG1	ILE	205	34.398	31.112	12.616	1.00	39.46
	ATOM	1543	CD1	ILE	205	34.250	30.158	11.425	1.00	39.34
15	ATOM	1544	C	ILE	205	32.527	29.215	15.440	1.00	41.34
	ATOM	1545	O	ILE	205	32.121	28.050	15.408	1.00	41.41
	ATOM	1546	N	SER	206	32.812	29.830	16.584	1.00	42.01
	ATOM	1547	CA	SER	206	32.683	29.112	17.849	1.00	43.71
	ATOM	1548	CB	SER	206	32.999	30.038	19.013	1.00	43.57
20	ATOM	1549	OG	SER	206	32.149	31.163	18.971	1.00	44.54
	ATOM	1550	C	SER	206	31.306	28.494	18.056	1.00	44.83
	ATOM	1551	O	SER	206	31.185	27.304	18.364	1.00	45.40
	ATOM	1552	N	CYS	207	30.260	29.291	17.894	1.00	46.32
	ATOM	1553	CA	CYS	207	28.912	28.764	18.079	1.00	48.14
25	ATOM	1554	CB	CYS	207	27.869	29.842	17.780	1.00	46.74
	ATOM	1555	SG	CYS	207	27.946	31.264	18.883	1.00	42.50
	ATOM	1556	C	CYS	207	28.666	27.551	17.186	1.00	50.79
	ATOM	1557	O	CYS	207	27.715	26.799	17.403	1.00	50.97
	ATOM	1558	N	TYR	208	29.533	27.361	16.190	1.00	53.91
30	ATOM	1559	CA	TYR	208	29.418	26.243	15.247	1.00	56.61
	ATOM	1560	CB	TYR	208	30.350	26.458	14.045	1.00	56.96
	ATOM	1561	CG	TYR	208	30.370	25.303	13.062	1.00	57.29
	ATOM	1562	CD1	TYR	208	29.307	25.090	12.182	1.00	57.54
	ATOM	1563	CE1	TYR	208	29.319	24.026	11.280	1.00	57.47
35	ATOM	1564	CD2	TYR	208	31.448	24.418	13.019	1.00	57.54
	ATOM	1565	CE2	TYR	208	31.468	23.350	12.125	1.00	57.60
	ATOM	1566	CZ	TYR	208	30.404	23.163	11.258	1.00	57.47
	ATOM	1567	OH	TYR	208	30.435	22.126	10.360	1.00	57.71
	ATOM	1568	C	TYR	208	29.705	24.867	15.854	1.00	58.12
40	ATOM	1569	O	TYR	208	28.874	23.960	15.773	1.00	58.61
	ATOM	1570	N	TYR	209	30.876	24.699	16.459	1.00	59.77
	ATOM	1571	CA	TYR	209	31.198	23.399	17.028	1.00	61.36
	ATOM	1572	CB	TYR	209	32.619	23.394	17.581	1.00	63.23
	ATOM	1573	CG	TYR	209	33.648	23.401	16.472	1.00	65.26
45	ATOM	1574	CD1	TYR	209	34.058	24.595	15.876	1.00	66.13
	ATOM	1575	CE1	TYR	209	34.959	24.594	14.807	1.00	67.31
	ATOM	1576	CD2	TYR	209	34.165	22.206	15.973	1.00	65.88
	ATOM	1577	CE2	TYR	209	35.062	22.193	14.906	1.00	66.79
	ATOM	1578	CZ	TYR	209	35.457	23.386	14.328	1.00	67.37
50	ATOM	1579	OH	TYR	209	36.350	23.370	13.277	1.00	67.62
	ATOM	1580	C	TYR	209	30.206	22.965	18.083	1.00	61.32
	ATOM	1581	O	TYR	209	30.048	21.771	18.336	1.00	61.19
	ATOM	1582	N	GLU	210	29.523	23.938	18.680	1.00	61.63
	ATOM	1583	CA	GLU	210	28.524	23.658	19.701	1.00	61.05
55	ATOM	1584	CB	GLU	210	28.444	24.808	20.706	1.00	62.29
	ATOM	1585	CG	GLU	210	27.539	24.499	21.884	1.00	65.45
	ATOM	1586	CD	GLU	210	27.716	25.463	23.050	1.00	67.38
	ATOM	1587	OE1	GLU	210	28.865	25.609	23.535	1.00	68.93
	ATOM	1588	OE2	GLU	210	26.707	26.065	23.488	1.00	67.92

Figure 4

	ATOM	1589	C	GLU	210	27.175	23.459	19.026	1.00	60.04
	ATOM	1590	O	GLU	210	26.255	22.901	19.618	1.00	59.93
	ATOM	1591	N	ASP	211	27.073	23.920	17.780	1.00	58.82
	ATOM	1592	CA	ASP	211	25.849	23.797	16.984	1.00	57.80
5	ATOM	1593	CB	ASP	211	24.804	24.824	17.441	1.00	58.16
	ATOM	1594	CG	ASP	211	23.504	24.730	16.653	1.00	58.25
	ATOM	1595	OD1	ASP	211	22.490	25.299	17.111	1.00	57.88
	ATOM	1596	OD2	ASP	211	23.495	24.096	15.572	1.00	58.65
	ATOM	1597	C	ASP	211	26.173	23.993	15.503	1.00	56.54
10	ATOM	1598	O	ASP	211	26.351	25.116	15.037	1.00	56.17
	ATOM	1599	N	HIS	212	26.234	22.884	14.773	1.00	55.81
	ATOM	1600	CA	HIS	212	26.577	22.884	13.351	1.00	55.26
	ATOM	1601	CB	HIS	212	26.699	21.442	12.852	1.00	57.87
	ATOM	1602	CG	HIS	212	27.816	20.678	13.493	1.00	61.52
15	ATOM	1603	CD2	HIS	212	27.815	19.527	14.205	1.00	62.63
	ATOM	1604	ND1	HIS	212	29.127	21.110	13.460	1.00	62.80
	ATOM	1605	CE1	HIS	212	29.884	20.258	14.127	1.00	63.70
	ATOM	1606	NE2	HIS	212	29.114	19.288	14.590	1.00	63.71
	ATOM	1607	C	HIS	212	25.665	23.656	12.412	1.00	53.29
20	ATOM	1608	O	HIS	212	26.014	23.883	11.251	1.00	52.77
	ATOM	1609	N	GLN	213	24.496	24.058	12.895	1.00	51.08
	ATOM	1610	CA	GLN	213	23.579	24.790	12.037	1.00	48.22
	ATOM	1611	CB	GLN	213	22.135	24.347	12.298	1.00	49.39
	ATOM	1612	CG	GLN	213	21.957	22.839	12.130	1.00	50.76
25	ATOM	1613	CD	GLN	213	20.507	22.410	11.965	1.00	51.82
	ATOM	1614	OE1	GLN	213	19.653	22.721	12.803	1.00	52.48
	ATOM	1615	NE2	GLN	213	20.223	21.679	10.883	1.00	51.72
	ATOM	1616	C	GLN	213	23.746	26.289	12.202	1.00	45.19
	ATOM	1617	O	GLN	213	22.978	27.077	11.654	1.00	45.00
30	ATOM	1618	N	CYS	214	24.759	26.686	12.957	1.00	41.87
	ATOM	1619	CA	CYS	214	25.015	28.105	13.122	1.00	39.08
	ATOM	1620	CB	CYS	214	25.907	28.386	14.332	1.00	39.18
	ATOM	1621	SG	CYS	214	26.281	30.175	14.542	1.00	40.32
	ATOM	1622	C	CYS	214	25.743	28.530	11.859	1.00	36.43
35	ATOM	1623	O	CYS	214	26.915	28.214	11.689	1.00	36.06
	ATOM	1624	N	GLU	215	25.046	29.223	10.967	1.00	33.00
	ATOM	1625	CA	GLU	215	25.664	29.672	9.736	1.00	30.60
	ATOM	1626	CB	GLU	215	25.056	28.960	8.541	1.00	31.95
	ATOM	1627	CG	GLU	215	25.289	27.466	8.561	1.00	33.57
40	ATOM	1628	CD	GLU	215	24.973	26.827	7.233	1.00	35.80
	ATOM	1629	OE1	GLU	215	25.719	27.094	6.264	1.00	37.32
	ATOM	1630	OE2	GLU	215	23.978	26.064	7.156	1.00	37.21
	ATOM	1631	C	GLU	215	25.518	31.162	9.563	1.00	28.84
	ATOM	1632	O	GLU	215	25.665	31.687	8.459	1.00	28.39
45	ATOM	1633	N	VAL	216	25.243	31.847	10.669	1.00	26.45
	ATOM	1634	CA	VAL	216	25.083	33.291	10.648	1.00	23.67
	ATOM	1635	CB	VAL	216	23.589	33.706	10.607	1.00	23.44
	ATOM	1636	CG1	VAL	216	23.485	35.214	10.492	1.00	22.72
	ATOM	1637	CG2	VAL	216	22.875	33.031	9.449	1.00	22.30
50	ATOM	1638	C	VAL	216	25.671	33.858	11.921	1.00	22.20
	ATOM	1639	O	VAL	216	25.444	33.328	13.006	1.00	22.86
	ATOM	1640	N	GLY	217	26.423	34.939	11.793	1.00	21.40
	ATOM	1641	CA	GLY	217	26.997	35.554	12.965	1.00	21.14
	ATOM	1642	C	GLY	217	26.524	36.994	13.022	1.00	22.30
55	ATOM	1643	O	GLY	217	26.432	37.677	11.983	1.00	22.05
	ATOM	1644	N	MSE	218	26.201	37.454	14.228	1.00	23.03
	ATOM	1645	CA	MSE	218	25.748	38.815	14.414	1.00	23.03
	ATOM	1646	CB	MSE	218	24.208	38.880	14.445	1.00	25.98
	ATOM	1647	CG	MSE	218	23.647	40.306	14.646	1.00	28.99

Figure 4

	ATOM	1648	SE	MSE	218	21.806	40.486	14.543	1.00 35.34
	ATOM	1649	CE	MSE	218	21.273	39.804	16.207	1.00 31.95
	ATOM	1650	C	MSE	218	26.320	39.405	15.694	1.00 21.99
	ATOM	1651	O	MSE	218	26.425	38.738	16.724	1.00 22.34
5	ATOM	1652	N	ILE	219	26.694	40.670	15.606	1.00 21.28
	ATOM	1653	CA	ILE	219	27.240	41.402	16.720	1.00 20.85
	ATOM	1654	CB	ILE	219	28.702	41.840	16.449	1.00 20.74
	ATOM	1655	CG2	ILE	219	29.164	42.757	17.558	1.00 19.65
	ATOM	1656	CG1	ILE	219	29.623	40.627	16.335	1.00 19.32
10	ATOM	1657	CD1	ILE	219	29.656	39.770	17.596	1.00 20.63
	ATOM	1658	C	ILE	219	26.413	42.676	16.838	1.00 21.47
	ATOM	1659	O	ILE	219	26.297	43.431	15.868	1.00 21.30
	ATOM	1660	N	VAL	220	25.823	42.908	18.003	1.00 21.91
	ATOM	1661	CA	VAL	220	25.059	44.135	18.224	1.00 22.49
15	ATOM	1662	CB	VAL	220	23.563	43.873	18.479	1.00 22.04
	ATOM	1663	CG1	VAL	220	22.815	45.183	18.425	1.00 21.50
	ATOM	1664	CG2	VAL	220	23.007	42.901	17.463	1.00 22.03
	ATOM	1665	C	VAL	220	25.650	44.775	19.477	1.00 23.27
	ATOM	1666	O	VAL	220	25.095	44.642	20.575	1.00 23.94
20	ATOM	1667	N	GLY	221	26.795	45.436	19.312	1.00 22.78
	ATOM	1668	CA	GLY	221	27.448	46.063	20.443	1.00 22.86
	ATOM	1669	C	GLY	221	27.728	47.509	20.138	1.00 23.75
	ATOM	1670	O	GLY	221	26.816	48.264	19.828	1.00 25.09
	ATOM	1671	N	THR	222	28.988	47.906	20.233	1.00 24.06
25	ATOM	1672	CA	THR	222	29.375	49.277	19.939	1.00 24.06
	ATOM	1673	CB	THR	222	30.893	49.423	19.960	1.00 24.59
	ATOM	1674	OG1	THR	222	31.377	49.051	21.258	1.00 26.00
	ATOM	1675	CG2	THR	222	31.299	50.860	19.640	1.00 24.67
	ATOM	1676	C	THR	222	28.888	49.530	18.533	1.00 24.09
30	ATOM	1677	O	THR	222	28.248	50.530	18.259	1.00 24.72
	ATOM	1678	N	GLY	223	29.211	48.597	17.646	1.00 24.40
	ATOM	1679	CA	GLY	223	28.790	48.686	16.262	1.00 24.65
	ATOM	1680	C	GLY	223	27.797	47.560	16.020	1.00 25.05
	ATOM	1681	O	GLY	223	27.478	46.779	16.936	1.00 25.80
35	ATOM	1682	N	CYS	224	27.298	47.453	14.798	1.00 24.73
	ATOM	1683	CA	CYS	224	26.338	46.405	14.504	1.00 24.18
	ATOM	1684	CB	CYS	224	24.928	46.958	14.682	1.00 24.47
	ATOM	1685	SG	CYS	224	23.640	45.925	13.998	1.00 25.11
	ATOM	1686	C	CYS	224	26.550	45.895	13.085	1.00 23.65
40	ATOM	1687	O	CYS	224	26.618	46.683	12.144	1.00 24.07
	ATOM	1688	N	ASN	225	26.650	44.578	12.941	1.00 23.06
	ATOM	1689	CA	ASN	225	26.883	43.963	11.638	1.00 23.27
	ATOM	1690	CB	ASN	225	28.346	44.230	11.210	1.00 26.15
	ATOM	1691	CG	ASN	225	28.831	43.296	10.098	1.00 27.94
45	ATOM	1692	OD1	ASN	225	28.271	43.265	8.997	1.00 29.23
	ATOM	1693	ND2	ASN	225	29.878	42.524	10.393	1.00 28.62
	ATOM	1694	C	ASN	225	26.603	42.459	11.740	1.00 21.80
	ATOM	1695	O	ASN	225	26.291	41.954	12.827	1.00 20.54
	ATOM	1696	N	ALA	226	26.709	41.759	10.610	1.00 19.99
50	ATOM	1697	CA	ALA	226	26.478	40.322	10.566	1.00 19.47
	ATOM	1698	CB	ALA	226	24.994	40.032	10.443	1.00 20.99
	ATOM	1699	C	ALA	226	27.194	39.723	9.378	1.00 18.72
	ATOM	1700	O	ALA	226	27.529	40.428	8.415	1.00 17.97
	ATOM	1701	N	CYS	227	27.404	38.415	9.439	1.00 18.36
55	ATOM	1702	CA	CYS	227	28.077	37.675	8.368	1.00 19.35
	ATOM	1703	CB	CYS	227	29.523	37.396	8.751	1.00 18.42
	ATOM	1704	SG	CYS	227	29.556	36.326	10.207	1.00 20.13
	ATOM	1705	C	CYS	227	27.331	36.352	8.291	1.00 19.81
	ATOM	1706	O	CYS	227	26.702	35.951	9.280	1.00 20.62

Figure 4

	ATOM	1707	N	TYR	228	27.402	35.668	7.148	1.00	20.49
	ATOM	1708	CA	TYR	228	26.705	34.384	6.989	1.00	20.56
	ATOM	1709	CB	TYR	228	25.242	34.633	6.624	1.00	17.90
	ATOM	1710	CG	TYR	228	25.096	35.134	5.204	1.00	15.65
5	ATOM	1711	CD1	TYR	228	24.922	34.249	4.145	1.00	15.81
	ATOM	1712	CE1	TYR	228	24.885	34.701	2.823	1.00	15.89
	ATOM	1713	CD2	TYR	228	25.221	36.483	4.913	1.00	15.28
	ATOM	1714	CE2	TYR	228	25.186	36.949	3.601	1.00	16.08
	ATOM	1715	CZ	TYR	228	25.022	36.051	2.564	1.00	16.76
10	ATOM	1716	OH	TYR	228	25.033	36.505	1.263	1.00	18.93
	ATOM	1717	C	TYR	228	27.345	33.539	5.887	1.00	22.19
	ATOM	1718	O	TYR	228	28.174	34.024	5.112	1.00	21.49
	ATOM	1719	N	MSE	229	26.928	32.278	5.808	1.00	24.74
	ATOM	1720	CA	MSE	229	27.438	31.349	4.808	1.00	26.69
15	ATOM	1721	CB	MSE	229	27.342	29.918	5.339	1.00	28.61
	ATOM	1722	CG	MSE	229	28.167	29.637	6.598	1.00	32.37
	ATOM	1723	SE	MSE	229	29.987	30.056	6.460	1.00	41.17
	ATOM	1724	CE	MSE	229	30.544	28.874	5.098	1.00	36.30
	ATOM	1725	C	MSE	229	26.663	31.470	3.481	1.00	27.83
20	ATOM	1726	O	MSE	229	25.535	30.994	3.363	1.00	28.02
	ATOM	1727	N	GLU	230	27.282	32.109	2.492	1.00	29.19
	ATOM	1728	CA	GLU	230	26.688	32.296	1.172	1.00	29.81
	ATOM	1729	CB	GLU	230	27.165	33.623	0.577	1.00	30.83
	ATOM	1730	CG	GLU	230	26.685	33.922	-0.843	1.00	32.33
25	ATOM	1731	CD	GLU	230	25.173	33.825	-0.989	1.00	34.04
	ATOM	1732	OE1	GLU	230	24.663	32.698	-1.222	1.00	34.43
	ATOM	1733	OE2	GLU	230	24.497	34.878	-0.858	1.00	33.65
	ATOM	1734	C	GLU	230	27.127	31.143	0.282	1.00	30.91
	ATOM	1735	O	GLU	230	27.958	30.319	0.685	1.00	30.80
30	ATOM	1736	N	GLU	231	26.562	31.078	-0.923	1.00	32.47
	ATOM	1737	CA	GLU	231	26.885	30.024	-1.883	1.00	34.04
	ATOM	1738	CB	GLU	231	25.668	29.696	-2.745	1.00	34.21
	ATOM	1739	CG	GLU	231	24.408	29.396	-1.979	1.00	34.89
	ATOM	1740	CD	GLU	231	24.452	28.054	-1.296	1.00	36.36
35	ATOM	1741	OE1	GLU	231	24.745	27.064	-2.002	1.00	36.80
	ATOM	1742	OE2	GLU	231	24.182	27.981	-0.067	1.00	36.72
	ATOM	1743	C	GLU	231	27.997	30.550	-2.777	1.00	35.65
	ATOM	1744	O	GLU	231	27.889	31.663	-3.304	1.00	35.42
	ATOM	1745	N	MSE	232	29.060	29.758	-2.952	1.00	37.13
40	ATOM	1746	CA	MSE	232	30.188	30.181	-3.780	1.00	38.19
	ATOM	1747	CB	MSE	232	31.191	29.036	-3.935	1.00	41.27
	ATOM	1748	CG	MSE	232	32.195	28.912	-2.765	1.00	45.40
	ATOM	1749	SE	MSE	232	33.237	30.431	-2.467	1.00	52.07
	ATOM	1750	CE	MSE	232	34.286	30.483	-3.969	1.00	48.20
45	ATOM	1751	C	MSE	232	29.694	30.664	-5.137	1.00	38.02
	ATOM	1752	O	MSE	232	30.179	31.656	-5.678	1.00	36.84
	ATOM	1753	N	GLN	233	28.698	29.970	-5.668	1.00	38.35
	ATOM	1754	CA	GLN	233	28.110	30.331	-6.948	1.00	38.79
	ATOM	1755	CB	GLN	233	26.954	29.373	-7.257	1.00	40.19
50	ATOM	1756	CG	GLN	233	25.658	30.041	-7.672	1.00	41.80
	ATOM	1757	CD	GLN	233	24.460	29.119	-7.510	1.00	43.22
	ATOM	1758	OE1	GLN	233	24.226	28.582	-6.424	1.00	44.27
	ATOM	1759	NE2	GLN	233	23.688	28.936	-8.586	1.00	43.87
	ATOM	1760	C	GLN	233	27.615	31.777	-6.936	1.00	38.45
55	ATOM	1761	O	GLN	233	27.495	32.407	-7.984	1.00	39.07
	ATOM	1762	N	ASN	234	27.329	32.313	-5.753	1.00	37.79
	ATOM	1763	CA	ASN	234	26.840	33.687	-5.668	1.00	36.56
	ATOM	1764	CB	ASN	234	25.657	33.771	-4.706	1.00	37.03
	ATOM	1765	CG	ASN	234	24.505	32.864	-5.119	1.00	36.83

Figure 4

	ATOM	1766	OD1	ASN	234	24.152	32.793	-6.299	1.00	36.50
	ATOM	1767	ND2	ASN	234	23.910	32.173	-4.146	1.00	36.25
	ATOM	1768	C	ASN	234	27.919	34.676	-5.250	1.00	35.71
	ATOM	1769	O	ASN	234	27.712	35.890	-5.301	1.00	35.11
5	ATOM	1770	N	VAL	235	29.069	34.156	-4.837	1.00	35.22
	ATOM	1771	CA	VAL	235	30.177	35.009	-4.439	1.00	34.85
	ATOM	1772	CB	VAL	235	31.056	34.321	-3.384	1.00	34.01
	ATOM	1773	CG1	VAL	235	31.949	35.343	-2.717	1.00	32.35
	ATOM	1774	CG2	VAL	235	30.185	33.576	-2.376	1.00	32.63
10	ATOM	1775	C	VAL	235	30.999	35.209	-5.706	1.00	35.79
	ATOM	1776	O	VAL	235	32.011	34.548	-5.910	1.00	35.65
	ATOM	1777	N	GLU	236	30.556	36.125	-6.556	1.00	37.55
	ATOM	1778	CA	GLU	236	31.220	36.383	-7.830	1.00	39.52
	ATOM	1779	CB	GLU	236	30.337	37.284	-8.701	1.00	39.67
15	ATOM	1780	CG	GLU	236	29.242	36.539	-9.448	1.00	41.02
	ATOM	1781	CD	GLU	236	28.214	37.467	-10.072	1.00	42.58
	ATOM	1782	OE1	GLU	236	28.607	38.529	-10.630	1.00	42.67
	ATOM	1783	OE2	GLU	236	27.009	37.121	-10.011	1.00	43.02
	ATOM	1784	C	GLU	236	32.631	36.961	-7.782	1.00	40.97
20	ATOM	1785	O	GLU	236	33.328	36.967	-8.803	1.00	42.27
	ATOM	1786	N	LEU	237	33.064	37.457	-6.628	1.00	41.32
	ATOM	1787	CA	LEU	237	34.408	38.017	-6.538	1.00	41.63
	ATOM	1788	CB	LEU	237	34.438	39.163	-5.537	1.00	41.68
	ATOM	1789	CG	LEU	237	33.545	40.367	-5.820	1.00	42.50
25	ATOM	1790	CD1	LEU	237	33.630	41.301	-4.623	1.00	44.17
	ATOM	1791	CD2	LEU	237	33.984	41.101	-7.085	1.00	42.46
	ATOM	1792	C	LEU	237	35.454	36.970	-6.148	1.00	42.43
	ATOM	1793	O	LEU	237	36.636	37.294	-6.010	1.00	42.30
	ATOM	1794	N	VAL	238	35.019	35.724	-5.967	1.00	42.96
30	ATOM	1795	CA	VAL	238	35.922	34.629	-5.606	1.00	43.89
	ATOM	1796	CB	VAL	238	35.917	34.380	-4.097	1.00	42.33
	ATOM	1797	CG1	VAL	238	36.722	33.136	-3.769	1.00	41.32
	ATOM	1798	CG2	VAL	238	36.503	35.578	-3.385	1.00	42.74
	ATOM	1799	C	VAL	238	35.520	33.337	-6.313	1.00	45.65
35	ATOM	1800	O	VAL	238	34.755	32.555	-5.770	1.00	46.15
	ATOM	1801	N	GLU	239	36.069	33.116	-7.510	1.00	47.60
	ATOM	1802	CA	GLU	239	35.769	31.947	-8.346	1.00	48.96
	ATOM	1803	CB	GLU	239	36.819	31.793	-9.448	1.00	51.17
	ATOM	1804	CG	GLU	239	37.000	33.026	-10.290	1.00	53.95
40	ATOM	1805	CD	GLU	239	37.817	34.066	-9.570	1.00	56.27
	ATOM	1806	OE1	GLU	239	39.070	33.982	-9.637	1.00	58.40
	ATOM	1807	OE2	GLU	239	37.211	34.950	-8.918	1.00	57.25
	ATOM	1808	C	GLU	239	35.599	30.594	-7.675	1.00	48.87
	ATOM	1809	O	GLU	239	36.272	30.274	-6.701	1.00	48.25
45	ATOM	1810	N	GLY	240	34.705	29.797	-8.252	1.00	49.09
	ATOM	1811	CA	GLY	240	34.412	28.469	-7.750	1.00	50.05
	ATOM	1812	C	GLY	240	32.967	28.418	-7.296	1.00	51.04
	ATOM	1813	O	GLY	240	32.482	29.379	-6.712	1.00	52.00
	ATOM	1814	N	ASP	241	32.259	27.332	-7.580	1.00	51.38
50	ATOM	1815	CA	ASP	241	30.882	27.214	-7.127	1.00	52.10
	ATOM	1816	CB	ASP	241	29.963	26.766	-8.252	1.00	52.95
	ATOM	1817	CG	ASP	241	30.186	27.534	-9.529	1.00	53.84
	ATOM	1818	OD1	ASP	241	30.046	28.779	-9.522	1.00	53.20
	ATOM	1819	OD2	ASP	241	30.496	26.875	-10.546	1.00	53.97
55	ATOM	1820	C	ASP	241	30.924	26.122	-6.083	1.00	52.90
	ATOM	1821	O	ASP	241	29.898	25.563	-5.701	1.00	53.59
	ATOM	1822	N	GLU	242	32.131	25.816	-5.626	1.00	53.45
	ATOM	1823	CA	GLU	242	32.325	24.760	-4.646	1.00	53.65
	ATOM	1824	CB	GLU	242	33.785	24.299	-4.670	1.00	55.19

Figure 4   35/63

	ATOM	1825	CG	GLU	242	34.056	23.062	-3.826	1.00	57.57
	ATOM	1826	CD	GLU	242	35.527	22.672	-3.811	1.00	58.85
	ATOM	1827	OE1	GLU	242	36.063	22.340	-4.893	1.00	59.63
	ATOM	1828	OE2	GLU	242	36.143	22.701	-2.717	1.00	59.85
5	ATOM	1829	C	GLU	242	31.933	25.159	-3.229	1.00	52.66
	ATOM	1830	O	GLU	242	32.469	26.113	-2.661	1.00	53.15
	ATOM	1831	N	GLY	243	30.987	24.418	-2.665	1.00	51.11
	ATOM	1832	CA	GLY	243	30.545	24.673	-1.305	1.00	48.74
	ATOM	1833	C	GLY	243	30.200	26.110	-0.967	1.00	46.87
10	ATOM	1834	O	GLY	243	29.879	26.917	-1.850	1.00	46.49
	ATOM	1835	N	ARG	244	30.288	26.421	0.326	1.00	44.89
	ATOM	1836	CA	ARG	244	29.967	27.748	0.838	1.00	43.27
	ATOM	1837	CB	ARG	244	28.852	27.639	1.873	1.00	42.24
	ATOM	1838	CG	ARG	244	27.571	27.040	1.339	1.00	42.16
15	ATOM	1839	CD	ARG	244	26.442	27.153	2.356	1.00	41.35
	ATOM	1840	NE	ARG	244	25.254	26.425	1.925	1.00	39.30
	ATOM	1841	CZ	ARG	244	24.702	25.446	2.630	1.00	39.15
	ATOM	1842	NH1	ARG	244	25.236	25.085	3.794	1.00	38.10
	ATOM	1843	NH2	ARG	244	23.627	24.821	2.168	1.00	38.77
20	ATOM	1844	C	ARG	244	31.121	28.524	1.465	1.00	42.34
	ATOM	1845	O	ARG	244	32.089	27.945	1.958	1.00	41.77
	ATOM	1846	N	MSE	245	30.990	29.849	1.446	1.00	42.07
	ATOM	1847	CA	MSE	245	31.977	30.745	2.042	1.00	41.32
	ATOM	1848	CB	MSE	245	32.846	31.391	0.974	1.00	42.25
25	ATOM	1849	CG	MSE	245	33.870	32.345	1.566	1.00	44.07
	ATOM	1850	SE	MSE	245	34.884	33.206	0.332	1.00	47.16
	ATOM	1851	CE	MSE	245	36.149	31.909	-0.005	1.00	44.40
	ATOM	1852	C	MSE	245	31.324	31.863	2.863	1.00	40.37
	ATOM	1853	O	MSE	245	30.525	32.644	2.338	1.00	40.13
30	ATOM	1854	N	CYS	246	31.664	31.940	4.148	1.00	38.95
	ATOM	1855	CA	CYS	246	31.125	32.990	5.001	1.00	37.00
	ATOM	1856	CB	CYS	246	31.794	32.953	6.376	1.00	37.69
	ATOM	1857	SG	CYS	246	31.231	34.229	7.567	1.00	38.96
	ATOM	1858	C	CYS	246	31.422	34.320	4.311	1.00	35.82
35	ATOM	1859	O	CYS	246	32.484	34.497	3.706	1.00	34.54
	ATOM	1860	N	VAL	247	30.466	35.240	4.388	1.00	34.51
	ATOM	1861	CA	VAL	247	30.591	36.566	3.782	1.00	32.46
	ATOM	1862	CB	VAL	247	29.609	36.751	2.588	1.00	32.34
	ATOM	1863	CG1	VAL	247	29.709	38.170	2.038	1.00	31.78
40	ATOM	1864	CG2	VAL	247	29.930	35.750	1.486	1.00	32.04
	ATOM	1865	C	VAL	247	30.239	37.580	4.863	1.00	32.03
	ATOM	1866	O	VAL	247	29.291	37.377	5.628	1.00	33.28
	ATOM	1867	N	ASN	248	31.011	38.657	4.931	1.00	29.34
	ATOM	1868	CA	ASN	248	30.792	39.699	5.917	1.00	27.36
45	ATOM	1869	CB	ASN	248	32.147	40.219	6.401	1.00	28.42
	ATOM	1870	CG	ASN	248	32.031	41.471	7.253	1.00	29.34
	ATOM	1871	OD1	ASN	248	30.975	41.774	7.816	1.00	29.82
	ATOM	1872	ND2	ASN	248	33.141	42.201	7.374	1.00	29.54
	ATOM	1873	C	ASN	248	29.983	40.798	5.257	1.00	27.10
50	ATOM	1874	O	ASN	248	30.531	41.618	4.503	1.00	26.98
	ATOM	1875	N	THR	249	28.679	40.823	5.544	1.00	26.01
	ATOM	1876	CA	THR	249	27.778	41.809	4.937	1.00	23.85
	ATOM	1877	CB	THR	249	26.325	41.634	5.424	1.00	23.81
	ATOM	1878	OG1	THR	249	26.228	42.100	6.775	1.00	25.10
55	ATOM	1879	CG2	THR	249	25.899	40.156	5.380	1.00	22.15
	ATOM	1880	C	THR	249	28.208	43.226	5.270	1.00	24.20
	ATOM	1881	O	THR	249	28.023	44.143	4.467	1.00	23.38
	ATOM	1882	N	GLU	250	28.777	43.406	6.462	1.00	24.31
	ATOM	1883	CA	GLU	250	29.219	44.733	6.891	1.00	23.61

Figure 4

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	ATOM	1884	CB	GLU	250	30.446	45.145	6.060	1.00	23.87
	ATOM	1885	CG	GLU	250	31.242	46.362	6.571	1.00	25.94
	ATOM	1886	CD	GLU	250	32.237	46.041	7.700	1.00	25.83
	ATOM	1887	OE1	GLU	250	32.728	44.893	7.813	1.00	25.67
5	ATOM	1888	OE2	GLU	250	32.552	46.960	8.473	1.00	26.46
	ATOM	1889	C	GLU	250	28.003	45.624	6.589	1.00	23.30
	ATOM	1890	O	GLU	250	28.110	46.648	5.896	1.00	23.33
	ATOM	1891	N	TRP	251	26.841	45.208	7.096	1.00	22.28
	ATOM	1892	CA	TRP	251	25.609	45.940	6.840	1.00	22.36
10	ATOM	1893	CB	TRP	251	24.376	45.077	7.133	1.00	20.65
	ATOM	1894	CG	TRP	251	24.133	44.726	8.543	1.00	18.29
	ATOM	1895	CD2	TRP	251	23.308	43.648	9.016	1.00	16.51
	ATOM	1896	CE2	TRP	251	23.279	43.725	10.424	1.00	15.08
	ATOM	1897	CE3	TRP	251	22.589	42.635	8.384	1.00	16.17
15	ATOM	1898	CD1	TRP	251	24.565	45.395	9.652	1.00	17.71
	ATOM	1899	NE1	TRP	251	24.051	44.795	10.795	1.00	17.10
	ATOM	1900	CZ2	TRP	251	22.567	42.830	11.201	1.00	14.23
	ATOM	1901	CZ3	TRP	251	21.872	41.737	9.171	1.00	15.72
	ATOM	1902	CH2	TRP	251	21.869	41.842	10.559	1.00	14.23
20	ATOM	1903	C	TRP	251	25.445	47.283	7.523	1.00	23.49
	ATOM	1904	O	TRP	251	24.541	48.044	7.167	1.00	23.95
	ATOM	1905	N	GLY	252	26.302	47.579	8.500	1.00	24.44
	ATOM	1906	CA	GLY	252	26.214	48.857	9.179	1.00	25.17
	ATOM	1907	C	GLY	252	26.195	49.979	8.152	1.00	26.19
25	ATOM	1908	O	GLY	252	25.715	51.086	8.429	1.00	26.19
	ATOM	1909	N	ALA	253	26.714	49.675	6.960	1.00	26.83
	ATOM	1910	CA	ALA	253	26.791	50.622	5.851	1.00	27.86
	ATOM	1911	CB	ALA	253	27.822	50.148	4.851	1.00	27.90
	ATOM	1912	C	ALA	253	25.448	50.834	5.144	1.00	28.52
30	ATOM	1913	O	ALA	253	25.249	51.834	4.448	1.00	27.73
	ATOM	1914	N	PHE	254	24.536	49.884	5.314	1.00	30.23
	ATOM	1915	CA	PHE	254	23.224	49.974	4.696	1.00	31.42
	ATOM	1916	CB	PHE	254	22.289	48.947	5.314	1.00	31.71
	ATOM	1917	CG	PHE	254	20.899	48.995	4.768	1.00	31.90
35	ATOM	1918	CD1	PHE	254	20.655	48.736	3.429	1.00	31.47
	ATOM	1919	CD2	PHE	254	19.824	49.273	5.600	1.00	32.95
	ATOM	1920	CE1	PHE	254	19.367	48.746	2.927	1.00	31.38
	ATOM	1921	CE2	PHE	254	18.518	49.285	5.096	1.00	32.69
	ATOM	1922	CZ	PHE	254	18.295	49.021	3.763	1.00	31.47
40	ATOM	1923	C	PHE	254	22.664	51.367	4.928	1.00	32.56
	ATOM	1924	O	PHE	254	22.638	51.839	6.064	1.00	33.19
	ATOM	1925	N	GLY	255	22.227	52.017	3.849	1.00	33.62
	ATOM	1926	CA	GLY	255	21.674	53.354	3.947	1.00	34.98
	ATOM	1927	C	GLY	255	22.673	54.429	3.565	1.00	36.85
45	ATOM	1928	O	GLY	255	22.317	55.604	3.424	1.00	36.70
	ATOM	1929	N	ASP	256	23.932	54.038	3.395	1.00	38.95
	ATOM	1930	CA	ASP	256	24.966	55.000	3.038	1.00	41.47
	ATOM	1931	CB	ASP	256	26.349	54.347	3.088	1.00	41.77
	ATOM	1932	CG	ASP	256	26.880	54.224	4.502	1.00	42.36
50	ATOM	1933	OD1	ASP	256	26.573	55.120	5.322	1.00	43.08
	ATOM	1934	OD2	ASP	256	27.617	53.251	4.791	1.00	42.28
	ATOM	1935	C	ASP	256	24.744	55.636	1.666	1.00	43.10
	ATOM	1936	O	ASP	256	25.489	56.533	1.261	1.00	44.08
	ATOM	1937	N	SER	257	23.729	55.171	0.946	1.00	44.19
55	ATOM	1938	CA	SER	257	23.427	55.738	-0.363	1.00	45.32
	ATOM	1939	CB	SER	257	23.714	54.713	-1.467	1.00	45.78
	ATOM	1940	OG	SER	257	22.845	53.601	-1.375	1.00	46.48
	ATOM	1941	C	SER	257	21.967	56.204	-0.423	1.00	45.41
	ATOM	1942	O	SER	257	21.378	56.316	-1.501	1.00	46.14

Figure 4

	ATOM	1943	N	GLY	258	21.393	56.466	0.751	1.00	45.52
	ATOM	1944	CA	GLY	258	20.018	56.933	0.835	1.00	45.22
	ATOM	1945	C	GLY	258	18.922	55.896	1.042	1.00	45.11
	ATOM	1946	O	GLY	258	17.745	56.253	1.068	1.00	45.45
5	ATOM	1947	N	GLU	259	19.284	54.627	1.205	1.00	44.67
	ATOM	1948	CA	GLU	259	18.288	53.572	1.380	1.00	44.04
	ATOM	1949	CB	GLU	259	18.954	52.187	1.415	1.00	44.23
	ATOM	1950	CG	GLU	259	19.952	51.916	0.295	1.00	44.88
	ATOM	1951	CD	GLU	259	21.318	52.552	0.548	1.00	45.53
10	ATOM	1952	OE1	GLU	259	21.381	53.785	0.753	1.00	44.98
	ATOM	1953	OE2	GLU	259	22.335	51.817	0.537	1.00	45.95
	ATOM	1954	C	GLU	259	17.462	53.749	2.647	1.00	43.91
	ATOM	1955	O	GLU	259	16.461	53.061	2.836	1.00	43.49
	ATOM	1956	N	LEU	260	17.875	54.661	3.520	1.00	43.87
15	ATOM	1957	CA	LEU	260	17.143	54.865	4.765	1.00	44.40
	ATOM	1958	CB	LEU	260	18.023	54.513	5.967	1.00	44.36
	ATOM	1959	CG	LEU	260	18.398	53.041	6.153	1.00	44.87
	ATOM	1960	CD1	LEU	260	19.315	52.879	7.369	1.00	44.30
	ATOM	1961	CD2	LEU	260	17.127	52.216	6.307	1.00	44.88
20	ATOM	1962	C	LEU	260	16.632	56.282	4.932	1.00	44.59
	ATOM	1963	O	LEU	260	15.744	56.534	5.749	1.00	44.72
	ATOM	1964	N	ASP	261	17.200	57.202	4.161	1.00	44.48
	ATOM	1965	CA	ASP	261	16.821	58.608	4.234	1.00	44.18
	ATOM	1966	CB	ASP	261	16.813	59.224	2.841	1.00	44.99
25	ATOM	1967	CG	ASP	261	18.192	59.310	2.247	1.00	46.23
	ATOM	1968	OD1	ASP	261	19.165	58.994	2.980	1.00	46.42
	ATOM	1969	OD2	ASP	261	18.296	59.697	1.055	1.00	46.79
	ATOM	1970	C	ASP	261	15.482	58.885	4.892	1.00	43.00
	ATOM	1971	O	ASP	261	15.415	59.592	5.898	1.00	42.63
30	ATOM	1972	N	GLU	262	14.424	58.317	4.320	1.00	41.88
	ATOM	1973	CA	GLU	262	13.070	58.525	4.810	1.00	41.00
	ATOM	1974	CB	GLU	262	12.088	57.744	3.940	1.00	41.65
	ATOM	1975	CG	GLU	262	12.249	56.254	3.999	1.00	43.54
	ATOM	1976	CD	GLU	262	11.359	55.562	2.996	1.00	45.44
35	ATOM	1977	OE1	GLU	262	11.715	55.561	1.800	1.00	47.21
	ATOM	1978	OE2	GLU	262	10.296	55.031	3.391	1.00	47.29
	ATOM	1979	C	GLU	262	12.830	58.211	6.286	1.00	39.99
	ATOM	1980	O	GLU	262	11.997	58.852	6.918	1.00	40.22
	ATOM	1981	N	PHE	263	13.545	57.238	6.845	1.00	38.83
40	ATOM	1982	CA	PHE	263	13.360	56.908	8.258	1.00	37.00
	ATOM	1983	CB	PHE	263	13.684	55.430	8.512	1.00	34.37
	ATOM	1984	CG	PHE	263	12.828	54.476	7.717	1.00	32.41
	ATOM	1985	CD1	PHE	263	13.366	53.753	6.660	1.00	30.67
	ATOM	1986	CD2	PHE	263	11.474	54.317	8.012	1.00	30.95
45	ATOM	1987	CE1	PHE	263	12.567	52.886	5.909	1.00	29.82
	ATOM	1988	CE2	PHE	263	10.667	53.450	7.261	1.00	28.87
	ATOM	1989	CZ	PHE	263	11.214	52.737	6.213	1.00	29.09
	ATOM	1990	C	PHE	263	14.197	57.797	9.190	1.00	36.78
	ATOM	1991	O	PHE	263	13.809	58.041	10.327	1.00	37.58
50	ATOM	1992	N	LEU	264	15.328	58.301	8.712	1.00	36.72
	ATOM	1993	CA	LEU	264	16.193	59.142	9.542	1.00	37.11
	ATOM	1994	CB	LEU	264	17.389	59.638	8.725	1.00	36.98
	ATOM	1995	CG	LEU	264	18.131	58.621	7.852	1.00	36.59
	ATOM	1996	CD1	LEU	264	19.233	59.346	7.077	1.00	35.39
55	ATOM	1997	CD2	LEU	264	18.701	57.503	8.717	1.00	35.46
	ATOM	1998	C	LEU	264	15.482	60.350	10.158	1.00	37.28
	ATOM	1999	O	LEU	264	14.879	61.148	9.451	1.00	38.03
	ATOM	2000	N	LEU	265	15.574	60.480	11.479	1.00	37.63
	ATOM	2001	CA	LEU	265	14.965	61.585	12.215	1.00	37.33

Figure 4

	ATOM	2002	CB	LEU	265	14.380	61.070	13.527	1.00	36.25
	ATOM	2003	CG	LEU	265	13.529	59.807	13.417	1.00	35.76
	ATOM	2004	CD1	LEU	265	13.157	59.295	14.808	1.00	35.17
	ATOM	2005	CD2	LEU	265	12.292	60.120	12.598	1.00	35.59
5	ATOM	2006	C	LEU	265	16.054	62.613	12.521	1.00	38.22
	ATOM	2007	O	LEU	265	17.239	62.285	12.486	1.00	38.34
	ATOM	2008	N	GLU	266	15.653	63.844	12.832	1.00	39.22
	ATOM	2009	CA	GLU	266	16.599	64.922	13.137	1.00	40.56
	ATOM	2010	CB	GLU	266	15.874	66.101	13.813	1.00	41.82
10	ATOM	2011	CG	GLU	266	15.277	65.777	15.196	1.00	44.28
	ATOM	2012	CD	GLU	266	14.612	66.974	15.886	1.00	44.95
	ATOM	2013	OE1	GLU	266	13.543	67.432	15.410	1.00	45.08
	ATOM	2014	OE2	GLU	266	15.163	67.452	16.910	1.00	45.53
	ATOM	2015	C	GLU	266	17.733	64.435	14.036	1.00	40.54
15	ATOM	2016	O	GLU	266	18.910	64.657	13.750	1.00	40.69
	ATOM	2017	N	TYR	267	17.366	63.760	15.121	1.00	40.61
	ATOM	2018	CA	TYR	267	18.342	63.234	16.062	1.00	40.30
	ATOM	2019	CB	TYR	267	17.639	62.364	17.110	1.00	39.44
	ATOM	2020	CG	TYR	267	16.216	62.784	17.423	1.00	38.98
20	ATOM	2021	CD1	TYR	267	15.134	61.967	17.066	1.00	38.66
	ATOM	2022	CE1	TYR	267	13.813	62.342	17.349	1.00	38.28
	ATOM	2023	CD2	TYR	267	15.943	63.995	18.075	1.00	38.72
	ATOM	2024	CE2	TYR	267	14.619	64.381	18.364	1.00	38.45
	ATOM	2025	CZ	TYR	267	13.564	63.548	17.996	1.00	38.30
25	ATOM	2026	OH	TYR	267	12.267	63.923	18.251	1.00	37.22
	ATOM	2027	C	TYR	267	19.381	62.403	15.296	1.00	40.27
	ATOM	2028	O	TYR	267	20.580	62.469	15.579	1.00	40.14
	ATOM	2029	N	ASP	268	18.909	61.626	14.324	1.00	40.61
	ATOM	2030	CA	ASP	268	19.781	60.790	13.511	1.00	40.87
30	ATOM	2031	CB	ASP	268	18.946	59.920	12.566	1.00	39.36
	ATOM	2032	CG	ASP	268	18.183	58.843	13.301	1.00	38.52
	ATOM	2033	OD1	ASP	268	18.819	58.118	14.082	1.00	39.79
	ATOM	2034	OD2	ASP	268	16.961	58.711	13.110	1.00	36.13
	ATOM	2035	C	ASP	268	20.764	61.643	12.712	1.00	41.97
35	ATOM	2036	O	ASP	268	21.956	61.339	12.667	1.00	42.91
	ATOM	2037	N	ARG	269	20.266	62.710	12.090	1.00	42.73
	ATOM	2038	CA	ARG	269	21.113	63.606	11.310	1.00	43.23
	ATOM	2039	CB	ARG	269	20.302	64.793	10.786	1.00	45.34
	ATOM	2040	CG	ARG	269	18.923	64.464	10.223	1.00	47.46
40	ATOM	2041	CD	ARG	269	19.000	63.819	8.864	1.00	49.22
	ATOM	2042	NE	ARG	269	17.667	63.552	8.337	1.00	52.67
	ATOM	2043	CZ	ARG	269	17.426	62.969	7.165	1.00	54.63
	ATOM	2044	NH1	ARG	269	18.436	62.591	6.386	1.00	55.41
	ATOM	2045	NH2	ARG	269	16.173	62.747	6.775	1.00	55.38
45	ATOM	2046	C	ARG	269	22.204	64.150	12.231	1.00	42.99
	ATOM	2047	O	ARG	269	23.400	63.999	11.977	1.00	43.63
	ATOM	2048	N	LEU	270	21.777	64.796	13.305	1.00	41.99
	ATOM	2049	CA	LEU	270	22.702	65.372	14.261	1.00	41.33
	ATOM	2050	CB	LEU	270	21.924	65.812	15.502	1.00	41.15
50	ATOM	2051	CG	LEU	270	21.004	67.002	15.217	1.00	40.34
	ATOM	2052	CD1	LEU	270	19.964	67.182	16.307	1.00	39.94
	ATOM	2053	CD2	LEU	270	21.879	68.237	15.084	1.00	40.26
	ATOM	2054	C	LEU	270	23.828	64.406	14.635	1.00	41.26
	ATOM	2055	O	LEU	270	25.009	64.762	14.553	1.00	41.76
55	ATOM	2056	N	VAL	271	23.462	63.188	15.030	1.00	40.24
	ATOM	2057	CA	VAL	271	24.443	62.177	15.415	1.00	40.08
	ATOM	2058	CB	VAL	271	23.776	60.838	15.730	1.00	40.42
	ATOM	2059	CG1	VAL	271	24.846	59.800	16.050	1.00	39.86
	ATOM	2060	CG2	VAL	271	22.796	61.000	16.891	1.00	40.86

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	ATOM	2061	C	VAL	271	25.477	61.903	14.329	1.00 40.51
	ATOM	2062	O	VAL	271	26.676	61.832	14.595	1.00 40.15
	ATOM	2063	N	ASP	272	24.998	61.730	13.103	1.00 40.78
	ATOM	2064	CA	ASP	272	25.866	61.447	11.977	1.00 40.36
5	ATOM	2065	CB	ASP	272	25.038	61.344	10.695	1.00 39.16
	ATOM	2066	CG	ASP	272	25.792	60.670	9.553	1.00 38.09
	ATOM	2067	OD1	ASP	272	26.821	60.000	9.807	1.00 36.54
	ATOM	2068	OD2	ASP	272	25.335	60.798	8.394	1.00 37.12
	ATOM	2069	C	ASP	272	26.901	62.544	11.849	1.00 40.88
10	ATOM	2070	O	ASP	272	28.099	62.297	11.953	1.00 40.75
	ATOM	2071	N	GLU	273	26.429	63.763	11.638	1.00 41.96
	ATOM	2072	CA	GLU	273	27.321	64.896	11.477	1.00 43.14
	ATOM	2073	CB	GLU	273	26.501	66.170	11.470	1.00 44.13
	ATOM	2074	CG	GLU	273	25.576	66.214	10.272	1.00 46.73
15	ATOM	2075	CD	GLU	273	24.629	67.388	10.308	1.00 48.40
	ATOM	2076	OE1	GLU	273	25.047	68.455	10.828	1.00 49.15
	ATOM	2077	OE2	GLU	273	23.482	67.241	9.811	1.00 48.64
	ATOM	2078	C	GLU	273	28.428	64.968	12.517	1.00 43.48
	ATOM	2079	O	GLU	273	29.575	65.279	12.187	1.00 43.59
20	ATOM	2080	N	SER	274	28.095	64.666	13.767	1.00 44.05
	ATOM	2081	CA	SER	274	29.089	64.702	14.837	1.00 44.54
	ATOM	2082	CB	SER	274	28.421	64.568	16.205	1.00 45.39
	ATOM	2083	OG	SER	274	27.496	65.611	16.424	1.00 48.14
	ATOM	2084	C	SER	274	30.106	63.582	14.694	1.00 44.23
25	ATOM	2085	O	SER	274	31.292	63.783	14.931	1.00 44.76
	ATOM	2086	N	SER	275	29.632	62.400	14.318	1.00 43.84
	ATOM	2087	CA	SER	275	30.489	61.227	14.162	1.00 43.42
	ATOM	2088	CB	SER	275	29.754	60.139	13.392	1.00 43.28
	ATOM	2089	OG	SER	275	29.758	60.444	12.010	1.00 42.94
30	ATOM	2090	C	SER	275	31.789	61.535	13.426	1.00 43.34
	ATOM	2091	O	SER	275	31.914	62.552	12.738	1.00 43.76
	ATOM	2092	N	ALA	276	32.756	60.639	13.570	1.00 42.68
	ATOM	2093	CA	ALA	276	34.034	60.805	12.906	1.00 42.98
	ATOM	2094	CB	ALA	276	35.108	60.015	13.639	1.00 42.92
35	ATOM	2095	C	ALA	276	33.930	60.319	11.465	1.00 43.23
	ATOM	2096	O	ALA	276	34.936	60.277	10.751	1.00 44.60
	ATOM	2097	N	ASN	277	32.722	59.949	11.039	1.00 42.10
	ATOM	2098	CA	ASN	277	32.517	59.447	9.691	1.00 40.87
	ATOM	2099	CB	ASN	277	32.615	57.927	9.685	1.00 41.63
40	ATOM	2100	CG	ASN	277	31.654	57.283	10.659	1.00 42.64
	ATOM	2101	OD1	ASN	277	30.670	57.898	11.067	1.00 43.50
	ATOM	2102	ND2	ASN	277	31.925	56.033	11.029	1.00 42.98
	ATOM	2103	C	ASN	277	31.178	59.865	9.104	1.00 40.57
	ATOM	2104	O	ASN	277	30.430	59.039	8.579	1.00 39.89
45	ATOM	2105	N	PRO	278	30.868	61.163	9.163	1.00 40.83
	ATOM	2106	CD	PRO	278	31.783	62.282	9.451	1.00 40.90
	ATOM	2107	CA	PRO	278	29.600	61.657	8.623	1.00 40.71
	ATOM	2108	CB	PRO	278	29.807	63.175	8.579	1.00 40.88
	ATOM	2109	CG	PRO	278	31.303	63.326	8.474	1.00 41.27
50	ATOM	2110	C	PRO	278	29.239	61.074	7.258	1.00 40.60
	ATOM	2111	O	PRO	278	29.949	61.284	6.270	1.00 40.71
	ATOM	2112	N	GLY	279	28.131	60.338	7.216	1.00 40.34
	ATOM	2113	CA	GLY	279	27.676	59.747	5.971	1.00 39.10
	ATOM	2114	C	GLY	279	27.904	58.252	5.828	1.00 38.94
55	ATOM	2115	O	GLY	279	27.315	57.635	4.952	1.00 39.74
	ATOM	2116	N	GLN	280	28.735	57.660	6.683	1.00 38.66
	ATOM	2117	CA	GLN	280	29.049	56.230	6.605	1.00 37.75
	ATOM	2118	CB	GLN	280	30.563	56.043	6.513	1.00 37.97
	ATOM	2119	CG	GLN	280	31.243	56.954	5.509	1.00 39.85

Figure 4

	ATOM	2120	CD	GLN	280	32.743	57.046	5.730	1.00	40.76
	ATOM	2121	OE1	GLN	280	33.465	56.058	5.587	1.00	41.39
	ATOM	2122	NE2	GLN	280	33.220	58.240	6.083	1.00	41.57
	ATOM	2123	C	GLN	280	28.553	55.455	7.817	1.00	36.99
5	ATOM	2124	O	GLN	280	28.645	55.939	8.941	1.00	37.89
	ATOM	2125	N	GLN	281	28.054	54.242	7.592	1.00	35.75
	ATOM	2126	CA	GLN	281	27.572	53.401	8.681	1.00	34.04
	ATOM	2127	CB	GLN	281	28.590	53.404	9.829	1.00	33.35
	ATOM	2128	CG	GLN	281	29.971	52.951	9.447	1.00	33.09
10	ATOM	2129	CD	GLN	281	29.967	51.576	8.800	1.00	34.44
	ATOM	2130	OE1	GLN	281	29.917	51.451	7.572	1.00	33.95
	ATOM	2131	NE2	GLN	281	30.000	50.529	9.630	1.00	34.63
	ATOM	2132	C	GLN	281	26.210	53.831	9.237	1.00	33.42
	ATOM	2133	O	GLN	281	25.895	53.530	10.390	1.00	34.87
15	ATOM	2134	N	LEU	282	25.395	54.511	8.436	1.00	31.53
	ATOM	2135	CA	LEU	282	24.098	54.992	8.913	1.00	29.87
	ATOM	2136	CB	LEU	282	23.345	55.685	7.777	1.00	30.15
	ATOM	2137	CG	LEU	282	24.030	56.871	7.085	1.00	30.41
	ATOM	2138	CD1	LEU	282	22.963	57.741	6.435	1.00	29.82
20	ATOM	2139	CD2	LEU	282	24.815	57.699	8.097	1.00	30.66
	ATOM	2140	C	LEU	282	23.191	53.949	9.578	1.00	28.70
	ATOM	2141	O	LEU	282	22.716	54.153	10.698	1.00	28.78
	ATOM	2142	N	TYR	283	22.935	52.841	8.894	1.00	27.35
	ATOM	2143	CA	TYR	283	22.095	51.793	9.461	1.00	26.53
25	ATOM	2144	CB	TYR	283	22.233	50.511	8.633	1.00	24.41
	ATOM	2145	CG	TYR	283	21.420	49.338	9.143	1.00	22.90
	ATOM	2146	CD1	TYR	283	20.021	49.413	9.210	1.00	21.94
	ATOM	2147	CE1	TYR	283	19.257	48.318	9.609	1.00	20.96
	ATOM	2148	CD2	TYR	283	22.038	48.129	9.503	1.00	21.53
30	ATOM	2149	CE2	TYR	283	21.279	47.030	9.907	1.00	20.87
	ATOM	2150	CZ	TYR	283	19.886	47.140	9.950	1.00	21.33
	ATOM	2151	OH	TYR	283	19.105	46.068	10.310	1.00	23.85
	ATOM	2152	C	TYR	283	22.567	51.532	10.891	1.00	27.12
	ATOM	2153	O	TYR	283	21.783	51.521	11.841	1.00	28.95
35	ATOM	2154	N	GLU	284	23.869	51.352	11.035	1.00	26.60
	ATOM	2155	CA	GLU	284	24.486	51.072	12.317	1.00	26.43
	ATOM	2156	CB	GLU	284	25.982	50.905	12.108	1.00	27.03
	ATOM	2157	CG	GLU	284	26.763	50.680	13.375	1.00	27.21
	ATOM	2158	CD	GLU	284	28.224	50.492	13.082	1.00	27.57
40	ATOM	2159	OE1	GLU	284	28.897	51.506	12.734	1.00	27.02
	ATOM	2160	OE2	GLU	284	28.670	49.319	13.185	1.00	26.30
	ATOM	2161	C	GLU	284	24.249	52.133	13.381	1.00	26.81
	ATOM	2162	O	GLU	284	24.197	51.826	14.582	1.00	26.06
	ATOM	2163	N	LYS	285	24.134	53.384	12.940	1.00	27.07
45	ATOM	2164	CA	LYS	285	23.926	54.502	13.860	1.00	27.39
	ATOM	2165	CB	LYS	285	24.339	55.825	13.186	1.00	25.99
	ATOM	2166	CG	LYS	285	25.840	56.012	13.132	1.00	24.13
	ATOM	2167	CD	LYS	285	26.235	57.110	12.179	1.00	23.29
	ATOM	2168	CE	LYS	285	27.755	57.193	12.052	1.00	22.03
50	ATOM	2169	NZ	LYS	285	28.142	58.198	11.027	1.00	21.72
	ATOM	2170	C	LYS	285	22.488	54.595	14.368	1.00	28.05
	ATOM	2171	O	LYS	285	22.086	55.615	14.941	1.00	28.61
	ATOM	2172	N	LEU	286	21.717	53.535	14.144	1.00	27.60
	ATOM	2173	CA	LEU	286	20.335	53.488	14.599	1.00	27.30
55	ATOM	2174	CB	LEU	286	19.399	53.157	13.435	1.00	28.57
	ATOM	2175	CG	LEU	286	19.375	54.167	12.279	1.00	30.25
	ATOM	2176	CD1	LEU	286	18.480	53.647	11.139	1.00	29.98
	ATOM	2177	CD2	LEU	286	18.863	55.507	12.780	1.00	29.35
	ATOM	2178	C	LEU	286	20.260	52.381	15.632	1.00	27.01

Figure 4

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	ATOM	2179	O	LEU	286	19.296	52.294	16.399	1.00	27.55
	ATOM	2180	N	ILE	287	21.306	51.554	15.645	1.00	26.00
	ATOM	2181	CA	ILE	287	21.415	50.399	16.532	1.00	24.38
	ATOM	2182	CB	ILE	287	21.551	49.141	15.715	1.00	23.92
5	ATOM	2183	CG2	ILE	287	21.470	47.919	16.628	1.00	22.70
	ATOM	2184	CG1	ILE	287	20.510	49.158	14.597	1.00	22.87
	ATOM	2185	CD1	ILE	287	20.676	48.042	13.607	1.00	22.79
	ATOM	2186	C	ILE	287	22.639	50.444	17.433	1.00	24.65
	ATOM	2187	O	ILE	287	22.550	50.255	18.644	1.00	23.54
10	ATOM	2188	N	GLY	288	23.791	50.668	16.810	1.00	25.94
	ATOM	2189	CA	GLY	288	25.060	50.714	17.519	1.00	26.86
	ATOM	2190	C	GLY	288	25.081	51.266	18.927	1.00	27.76
	ATOM	2191	O	GLY	288	24.697	52.412	19.164	1.00	28.19
	ATOM	2192	N	GLY	289	25.554	50.445	19.860	1.00	28.95
15	ATOM	2193	CA	GLY	289	25.656	50.856	21.249	1.00	30.54
	ATOM	2194	C	GLY	289	26.632	52.007	21.407	1.00	31.92
	ATOM	2195	O	GLY	289	26.930	52.442	22.509	1.00	32.56
	ATOM	2196	N	LYS	290	27.133	52.504	20.291	1.00	32.83
	ATOM	2197	CA	LYS	290	28.067	53.607	20.296	1.00	33.99
20	ATOM	2198	CB	LYS	290	29.104	53.373	19.191	1.00	35.04
	ATOM	2199	CG	LYS	290	29.858	54.598	18.665	1.00	36.71
	ATOM	2200	CD	LYS	290	31.032	54.996	19.551	1.00	38.80
	ATOM	2201	CE	LYS	290	31.936	56.011	18.839	1.00	39.77
	ATOM	2202	NZ	LYS	290	32.864	56.707	19.787	1.00	41.04
25	ATOM	2203	C	LYS	290	27.278	54.880	20.035	1.00	34.58
	ATOM	2204	O	LYS	290	27.810	55.984	20.138	1.00	35.79
	ATOM	2205	N	TYR	291	26.001	54.734	19.708	1.00	33.80
	ATOM	2206	CA	TYR	291	25.196	55.907	19.406	1.00	33.61
	ATOM	2207	CB	TYR	291	25.010	56.046	17.892	1.00	33.22
30	ATOM	2208	CG	TYR	291	26.256	55.752	17.084	1.00	33.77
	ATOM	2209	CD1	TYR	291	26.659	54.435	16.838	1.00	34.23
	ATOM	2210	CE1	TYR	291	27.789	54.155	16.065	1.00	34.17
	ATOM	2211	CD2	TYR	291	27.021	56.783	16.542	1.00	33.61
	ATOM	2212	CE2	TYR	291	28.150	56.515	15.773	1.00	33.54
35	ATOM	2213	CZ	TYR	291	28.528	55.200	15.532	1.00	33.76
	ATOM	2214	OH	TYR	291	29.620	54.928	14.729	1.00	34.36
	ATOM	2215	C	TYR	291	23.836	55.874	20.070	1.00	33.11
	ATOM	2216	O	TYR	291	23.069	56.828	19.975	1.00	32.86
	ATOM	2217	N	MSE	292	23.521	54.778	20.737	1.00	33.27
40	ATOM	2218	CA	MSE	292	22.230	54.699	21.389	1.00	33.18
	ATOM	2219	CB	MSE	292	22.066	53.349	22.062	1.00	33.77
	ATOM	2220	CG	MSE	292	20.639	52.975	22.314	1.00	35.15
	ATOM	2221	SE	MSE	292	20.564	51.230	22.803	1.00	41.54
	ATOM	2222	CE	MSE	292	20.269	50.385	21.171	1.00	35.91
45	ATOM	2223	C	MSE	292	22.148	55.818	22.423	1.00	32.97
	ATOM	2224	O	MSE	292	21.227	56.637	22.400	1.00	33.49
	ATOM	2225	N	GLY	293	23.131	55.861	23.315	1.00	32.96
	ATOM	2226	CA	GLY	293	23.151	56.892	24.334	1.00	32.25
	ATOM	2227	C	GLY	293	23.067	58.290	23.750	1.00	32.18
50	ATOM	2228	O	GLY	293	22.307	59.126	24.241	1.00	33.24
	ATOM	2229	N	GLU	294	23.835	58.560	22.702	1.00	31.47
	ATOM	2230	CA	GLU	294	23.809	59.883	22.096	1.00	31.38
	ATOM	2231	CB	GLU	294	24.875	59.971	21.008	1.00	33.29
	ATOM	2232	CG	GLU	294	24.986	61.321	20.304	1.00	34.67
55	ATOM	2233	CD	GLU	294	25.227	62.474	21.257	1.00	35.80
	ATOM	2234	OE1	GLU	294	25.708	62.244	22.389	1.00	36.49
	ATOM	2235	OE2	GLU	294	24.946	63.623	20.858	1.00	37.16
	ATOM	2236	C	GLU	294	22.428	60.192	21.521	1.00	30.62
	ATOM	2237	O	GLU	294	21.919	61.305	21.664	1.00	30.94

Figure 4

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	ATOM	2238	N	LEU	295	21.818	59.204	20.878	1.00	29.56
	ATOM	2239	CA	LEU	295	20.495	59.392	20.303	1.00	29.24
	ATOM	2240	CB	LEU	295	20.030	58.112	19.589	1.00	27.27
	ATOM	2241	CG	LEU	295	20.389	58.007	18.099	1.00	25.46
5	ATOM	2242	CD1	LEU	295	19.979	56.668	17.522	1.00	21.87
	ATOM	2243	CD2	LEU	295	19.677	59.136	17.352	1.00	25.71
	ATOM	2244	C	LEU	295	19.497	59.787	21.388	1.00	29.98
	ATOM	2245	O	LEU	295	18.587	60.573	21.156	1.00	30.19
	ATOM	2246	N	VAL	296	19.665	59.250	22.585	1.00	31.23
10	ATOM	2247	CA	VAL	296	18.745	59.590	23.657	1.00	32.87
	ATOM	2248	CB	VAL	296	18.890	58.623	24.831	1.00	32.48
	ATOM	2249	CG1	VAL	296	17.827	58.899	25.868	1.00	32.99
	ATOM	2250	CG2	VAL	296	18.762	57.198	24.323	1.00	33.56
	ATOM	2251	C	VAL	296	19.020	61.025	24.122	1.00	33.74
15	ATOM	2252	O	VAL	296	18.086	61.778	24.431	1.00	33.68
	ATOM	2253	N	ARG	297	20.296	61.409	24.145	1.00	34.02
	ATOM	2254	CA	ARG	297	20.659	62.757	24.563	1.00	35.34
	ATOM	2255	CB	ARG	297	22.147	63.008	24.342	1.00	34.89
	ATOM	2256	CG	ARG	297	22.940	63.279	25.609	1.00	35.27
20	ATOM	2257	CD	ARG	297	23.791	64.525	25.454	1.00	35.98
	ATOM	2258	NE	ARG	297	24.226	64.700	24.074	1.00	37.11
	ATOM	2259	CZ	ARG	297	24.476	65.878	23.513	1.00	37.43
	ATOM	2260	NH1	ARG	297	24.348	66.994	24.226	1.00	38.45
	ATOM	2261	NH2	ARG	297	24.809	65.944	22.229	1.00	36.61
25	ATOM	2262	C	ARG	297	19.870	63.766	23.747	1.00	36.07
	ATOM	2263	O	ARG	297	19.103	64.574	24.285	1.00	36.76
	ATOM	2264	N	LEU	298	20.063	63.699	22.437	1.00	36.93
	ATOM	2265	CA	LEU	298	19.407	64.596	21.500	1.00	37.55
	ATOM	2266	CB	LEU	298	19.768	64.178	20.077	1.00	37.28
30	ATOM	2267	CG	LEU	298	21.272	64.065	19.816	1.00	36.13
	ATOM	2268	CD1	LEU	298	21.478	63.784	18.341	1.00	36.85
	ATOM	2269	CD2	LEU	298	21.991	65.356	20.218	1.00	35.02
	ATOM	2270	C	LEU	298	17.892	64.633	21.670	1.00	38.53
	ATOM	2271	O	LEU	298	17.276	65.708	21.618	1.00	38.44
35	ATOM	2272	N	VAL	299	17.289	63.462	21.866	1.00	39.23
	ATOM	2273	CA	VAL	299	15.839	63.389	22.054	1.00	40.08
	ATOM	2274	CB	VAL	299	15.349	61.932	22.110	1.00	39.44
	ATOM	2275	CG1	VAL	299	13.844	61.892	22.385	1.00	37.91
	ATOM	2276	CG2	VAL	299	15.676	61.240	20.802	1.00	38.72
40	ATOM	2277	C	VAL	299	15.435	64.087	23.350	1.00	40.94
	ATOM	2278	O	VAL	299	14.321	64.612	23.461	1.00	41.66
	ATOM	2279	N	LEU	300	16.337	64.091	24.328	1.00	41.41
	ATOM	2280	CA	LEU	300	16.043	64.737	25.600	1.00	42.31
	ATOM	2281	CB	LEU	300	16.973	64.224	26.713	1.00	41.48
45	ATOM	2282	CG	LEU	300	16.943	62.766	27.206	1.00	40.38
	ATOM	2283	CD1	LEU	300	17.677	62.711	28.545	1.00	40.14
	ATOM	2284	CD2	LEU	300	15.517	62.251	27.380	1.00	38.74
	ATOM	2285	C	LEU	300	16.204	66.251	25.444	1.00	43.44
	ATOM	2286	O	LEU	300	15.304	67.020	25.806	1.00	43.84
50	ATOM	2287	N	LEU	301	17.346	66.675	24.898	1.00	43.90
	ATOM	2288	CA	LEU	301	17.603	68.100	24.707	1.00	43.85
	ATOM	2289	CB	LEU	301	18.895	68.335	23.919	1.00	43.20
	ATOM	2290	CG	LEU	301	20.211	67.969	24.613	1.00	43.48
	ATOM	2291	CD1	LEU	301	21.385	68.372	23.730	1.00	43.37
55	ATOM	2292	CD2	LEU	301	20.307	68.675	25.955	1.00	43.71
	ATOM	2293	C	LEU	301	16.444	68.738	23.969	1.00	44.11
	ATOM	2294	O	LEU	301	16.068	69.875	24.254	1.00	44.38
	ATOM	2295	N	ARG	302	15.863	68.007	23.025	1.00	44.45
	ATOM	2296	CA	ARG	302	14.753	68.571	22.280	1.00	45.04

Figure 4

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	ATOM	2297	CB	ARG	302	14.296	67.660	21.148	1.00	45.49
	ATOM	2298	CG	ARG	302	13.082	68.256	20.468	1.00	45.91
	ATOM	2299	CD	ARG	302	12.391	67.327	19.514	1.00	46.45
	ATOM	2300	NE	ARG	302	11.194	67.985	19.007	1.00	47.37
5	ATOM	2301	CZ	ARG	302	10.423	67.503	18.043	1.00	48.12
	ATOM	2302	NH1	ARG	302	10.719	66.344	17.466	1.00	48.80
	ATOM	2303	NH2	ARG	302	9.357	68.190	17.657	1.00	47.77
	ATOM	2304	C	ARG	302	13.577	68.807	23.196	1.00	45.13
	ATOM	2305	O	ARG	302	12.982	69.885	23.198	1.00	45.57
10	ATOM	2306	N	LEU	303	13.228	67.787	23.966	1.00	45.14
	ATOM	2307	CA	LEU	303	12.113	67.918	24.883	1.00	45.18
	ATOM	2308	CB	LEU	303	11.952	66.624	25.695	1.00	44.02
	ATOM	2309	CG	LEU	303	11.495	65.427	24.846	1.00	42.43
	ATOM	2310	CD1	LEU	303	11.365	64.162	25.690	1.00	41.06
15	ATOM	2311	CD2	LEU	303	10.154	65.784	24.207	1.00	41.96
	ATOM	2312	C	LEU	303	12.359	69.133	25.783	1.00	45.83
	ATOM	2313	O	LEU	303	11.444	69.919	26.044	1.00	45.85
	ATOM	2314	N	VAL	304	13.599	69.302	26.232	1.00	46.44
	ATOM	2315	CA	VAL	304	13.943	70.440	27.085	1.00	47.76
20	ATOM	2316	CB	VAL	304	15.443	70.426	27.496	1.00	47.79
	ATOM	2317	CG1	VAL	304	15.866	71.815	27.996	1.00	46.89
	ATOM	2318	CG2	VAL	304	15.678	69.386	28.581	1.00	47.81
	ATOM	2319	C	VAL	304	13.666	71.764	26.371	1.00	48.44
	ATOM	2320	O	VAL	304	12.899	72.596	26.861	1.00	48.95
25	ATOM	2321	N	ASP	305	14.297	71.946	25.212	1.00	48.52
	ATOM	2322	CA	ASP	305	14.143	73.165	24.432	1.00	48.31
	ATOM	2323	CB	ASP	305	14.968	73.067	23.143	1.00	49.45
	ATOM	2324	CG	ASP	305	16.441	72.715	23.412	1.00	51.00
	ATOM	2325	OD1	ASP	305	17.056	73.323	24.317	1.00	50.99
30	ATOM	2326	OD2	ASP	305	16.994	71.834	22.715	1.00	51.84
	ATOM	2327	C	ASP	305	12.677	73.460	24.122	1.00	47.77
	ATOM	2328	O	ASP	305	12.341	74.541	23.641	1.00	48.22
	ATOM	2329	N	GLU	306	11.799	72.505	24.407	1.00	46.84
	ATOM	2330	CA	GLU	306	10.378	72.713	24.176	1.00	46.34
35	ATOM	2331	CB	GLU	306	9.831	71.683	23.184	1.00	46.20
	ATOM	2332	CG	GLU	306	9.866	72.216	21.761	1.00	48.15
	ATOM	2333	CD	GLU	306	9.571	71.175	20.692	1.00	49.26
	ATOM	2334	OE1	GLU	306	8.514	70.499	20.768	1.00	50.03
	ATOM	2335	OE2	GLU	306	10.398	71.049	19.759	1.00	49.62
40	ATOM	2336	C	GLU	306	9.635	72.661	25.493	1.00	45.99
	ATOM	2337	O	GLU	306	8.459	72.331	25.550	1.00	45.90
	ATOM	2338	N	ASN	307	10.350	72.997	26.560	1.00	46.00
	ATOM	2339	CA	ASN	307	9.787	73.029	27.902	1.00	45.60
	ATOM	2340	CB	ASN	307	9.033	74.342	28.094	1.00	46.42
45	ATOM	2341	CG	ASN	307	9.971	75.531	28.224	1.00	46.98
	ATOM	2342	OD1	ASN	307	10.435	75.849	29.321	1.00	47.63
	ATOM	2343	ND2	ASN	307	10.273	76.181	27.102	1.00	46.93
	ATOM	2344	C	ASN	307	8.886	71.853	28.246	1.00	45.05
	ATOM	2345	O	ASN	307	7.812	72.029	28.829	1.00	45.19
50	ATOM	2346	N	LEU	308	9.336	70.650	27.900	1.00	44.24
	ATOM	2347	CA	LEU	308	8.575	69.439	28.180	1.00	43.28
	ATOM	2348	CB	LEU	308	8.376	68.637	26.893	1.00	43.27
	ATOM	2349	CG	LEU	308	7.070	68.825	26.115	1.00	44.09
	ATOM	2350	CD1	LEU	308	6.765	70.294	25.935	1.00	44.22
55	ATOM	2351	CD2	LEU	308	7.182	68.139	24.760	1.00	43.94
	ATOM	2352	C	LEU	308	9.287	68.570	29.205	1.00	42.96
	ATOM	2353	O	LEU	308	8.688	67.660	29.775	1.00	42.27
	ATOM	2354	N	LEU	309	10.560	68.868	29.448	1.00	43.49
	ATOM	2355	CA	LEU	309	11.368	68.077	30.371	1.00	44.85

Figure 4

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	ATOM	2356	CB	LEU	309	12.030	66.936	29.581	1.00	43.53
	ATOM	2357	CG	LEU	309	12.958	65.925	30.254	1.00	42.07
	ATOM	2358	CD1	LEU	309	12.235	65.226	31.390	1.00	40.83
	ATOM	2359	CD2	LEU	309	13.416	64.913	29.212	1.00	42.11
5	ATOM	2360	C	LEU	309	12.436	68.900	31.108	1.00	46.21
	ATOM	2361	O	LEU	309	13.074	69.777	30.518	1.00	46.04
	ATOM	2362	N	PHE	310	12.625	68.601	32.397	1.00	47.92
	ATOM	2363	CA	PHE	310	13.608	69.293	33.238	1.00	49.25
	ATOM	2364	CB	PHE	310	15.013	69.093	32.666	1.00	48.20
10	ATOM	2365	CG	PHE	310	15.438	67.650	32.590	1.00	47.06
	ATOM	2366	CD1	PHE	310	16.338	67.228	31.615	1.00	46.24
	ATOM	2367	CD2	PHE	310	14.947	66.715	33.497	1.00	46.63
	ATOM	2368	CE1	PHE	310	16.740	65.903	31.540	1.00	45.74
	ATOM	2369	CE2	PHE	310	15.344	65.385	33.433	1.00	46.27
15	ATOM	2370	CZ	PHE	310	16.243	64.978	32.451	1.00	45.93
	ATOM	2371	C	PHE	310	13.292	70.785	33.345	1.00	51.16
	ATOM	2372	O	PHE	310	14.185	71.616	33.561	1.00	50.84
	ATOM	2373	N	HIS	311	12.009	71.109	33.183	1.00	53.40
	ATOM	2374	CA	HIS	311	11.529	72.482	33.262	1.00	55.80
20	ATOM	2375	CB	HIS	311	11.744	73.012	34.683	1.00	57.57
	ATOM	2376	CG	HIS	311	11.212	72.098	35.745	1.00	59.78
	ATOM	2377	CD2	HIS	311	11.848	71.363	36.689	1.00	60.29
	ATOM	2378	ND1	HIS	311	9.867	71.815	35.879	1.00	60.36
	ATOM	2379	CE1	HIS	311	9.699	70.944	36.860	1.00	60.99
25	ATOM	2380	NE2	HIS	311	10.885	70.654	37.368	1.00	60.85
	ATOM	2381	C	HIS	311	12.214	73.384	32.236	1.00	56.24
	ATOM	2382	O	HIS	311	12.288	74.608	32.415	1.00	56.87
	ATOM	2383	N	GLY	312	12.705	72.772	31.159	1.00	55.96
	ATOM	2384	CA	GLY	312	13.366	73.522	30.109	1.00	55.87
30	ATOM	2385	C	GLY	312	14.820	73.804	30.420	1.00	56.16
	ATOM	2386	O	GLY	312	15.563	74.264	29.562	1.00	56.58
	ATOM	2387	N	GLU	313	15.235	73.519	31.646	1.00	56.52
	ATOM	2388	CA	GLU	313	16.612	73.765	32.048	1.00	57.69
	ATOM	2389	CB	GLU	313	16.621	74.379	33.447	1.00	59.84
35	ATOM	2390	CG	GLU	313	15.849	75.698	33.515	1.00	63.16
	ATOM	2391	CD	GLU	313	15.388	76.061	34.925	1.00	65.16
	ATOM	2392	OE1	GLU	313	14.554	75.315	35.503	1.00	66.01
	ATOM	2393	OE2	GLU	313	15.858	77.096	35.455	1.00	66.34
	ATOM	2394	C	GLU	313	17.439	72.484	32.011	1.00	57.06
40	ATOM	2395	O	GLU	313	17.155	71.529	32.728	1.00	57.01
	ATOM	2396	N	ALA	314	18.463	72.472	31.169	1.00	56.56
	ATOM	2397	CA	ALA	314	19.316	71.305	31.029	1.00	56.76
	ATOM	2398	CB	ALA	314	19.454	70.939	29.557	1.00	56.47
	ATOM	2399	C	ALA	314	20.699	71.490	31.643	1.00	56.94
45	ATOM	2400	O	ALA	314	21.310	72.558	31.527	1.00	57.46
	ATOM	2401	N	SER	315	21.183	70.422	32.276	1.00	56.73
	ATOM	2402	CA	SER	315	22.487	70.383	32.932	1.00	56.15
	ATOM	2403	CB	SER	315	22.666	69.029	33.624	1.00	56.44
	ATOM	2404	OG	SER	315	23.981	68.868	34.130	1.00	57.39
50	ATOM	2405	C	SER	315	23.673	70.627	32.003	1.00	56.00
	ATOM	2406	O	SER	315	23.595	70.416	30.793	1.00	55.42
	ATOM	2407	N	GLU	316	24.776	71.070	32.598	1.00	56.67
	ATOM	2408	CA	GLU	316	26.012	71.346	31.875	1.00	57.46
	ATOM	2409	CB	GLU	316	27.111	71.754	32.860	1.00	58.71
55	ATOM	2410	CG	GLU	316	28.458	72.050	32.206	1.00	60.34
	ATOM	2411	CD	GLU	316	28.442	73.343	31.406	1.00	61.64
	ATOM	2412	OE1	GLU	316	28.288	74.420	32.031	1.00	62.41
	ATOM	2413	OE2	GLU	316	28.574	73.280	30.160	1.00	61.76
	ATOM	2414	C	GLU	316	26.442	70.078	31.161	1.00	57.35

Figure 4

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	ATOM	2415	O	GLU	316	26.770	70.088	29.972	1.00	57.68
	ATOM	2416	N	GLN	317	26.439	68.988	31.920	1.00	56.84
	ATOM	2417	CA	GLN	317	26.817	67.677	31.427	1.00	56.23
	ATOM	2418	CB	GLN	317	26.760	66.669	32.580	1.00	55.93
5	ATOM	2419	CG	GLN	317	27.504	67.113	33.840	1.00	55.46
	ATOM	2420	CD	GLN	317	27.063	66.355	35.085	1.00	55.01
	ATOM	2421	OE1	GLN	317	27.246	65.140	35.194	1.00	54.83
	ATOM	2422	NE2	GLN	317	26.468	67.074	36.029	1.00	54.68
	ATOM	2423	C	GLN	317	25.902	67.210	30.290	1.00	56.37
10	ATOM	2424	O	GLN	317	26.376	66.634	29.312	1.00	56.16
	ATOM	2425	N	LEU	318	24.599	67.476	30.412	1.00	56.41
	ATOM	2426	CA	LEU	318	23.616	67.043	29.413	1.00	56.48
	ATOM	2427	CB	LEU	318	22.190	67.333	29.890	1.00	55.59
	ATOM	2428	CG	LEU	318	21.084	66.700	29.034	1.00	54.71
15	ATOM	2429	CD1	LEU	318	21.090	65.191	29.231	1.00	53.88
	ATOM	2430	CD2	LEU	318	19.731	67.268	29.422	1.00	54.28
	ATOM	2431	C	LEU	318	23.784	67.621	28.017	1.00	56.99
	ATOM	2432	O	LEU	318	23.692	66.893	27.029	1.00	57.21
	ATOM	2433	N	ARG	319	24.011	68.924	27.919	1.00	57.16
20	ATOM	2434	CA	ARG	319	24.177	69.530	26.606	1.00	57.68
	ATOM	2435	CB	ARG	319	23.870	71.026	26.690	1.00	59.32
	ATOM	2436	CG	ARG	319	22.420	71.284	27.105	1.00	62.20
	ATOM	2437	CD	ARG	319	22.125	72.743	27.401	1.00	64.53
	ATOM	2438	NE	ARG	319	20.758	72.927	27.892	1.00	66.89
25	ATOM	2439	CZ	ARG	319	20.297	74.055	28.433	1.00	68.29
	ATOM	2440	NH1	ARG	319	21.096	75.112	28.555	1.00	68.30
	ATOM	2441	NH2	ARG	319	19.034	74.127	28.851	1.00	68.25
	ATOM	2442	C	ARG	319	25.587	69.278	26.081	1.00	57.09
	ATOM	2443	O	ARG	319	26.049	69.951	25.160	1.00	57.05
30	ATOM	2444	N	THR	320	26.246	68.277	26.667	1.00	56.25
	ATOM	2445	CA	THR	320	27.612	67.888	26.318	1.00	55.15
	ATOM	2446	CB	THR	320	28.478	67.836	27.589	1.00	54.85
	ATOM	2447	OG1	THR	320	28.601	69.158	28.133	1.00	54.94
	ATOM	2448	CG2	THR	320	29.854	67.262	27.287	1.00	54.63
35	ATOM	2449	C	THR	320	27.689	66.524	25.613	1.00	55.04
	ATOM	2450	O	THR	320	27.476	65.480	26.229	1.00	55.13
	ATOM	2451	N	ARG	321	28.017	66.536	24.326	1.00	54.38
	ATOM	2452	CA	ARG	321	28.106	65.304	23.545	1.00	54.36
	ATOM	2453	CB	ARG	321	28.841	65.586	22.236	1.00	56.05
40	ATOM	2454	CG	ARG	321	28.153	66.651	21.402	1.00	59.03
	ATOM	2455	CD	ARG	321	28.943	67.013	20.156	1.00	61.60
	ATOM	2456	NE	ARG	321	28.331	68.123	19.426	1.00	63.68
	ATOM	2457	CZ	ARG	321	28.909	68.753	18.406	1.00	65.43
	ATOM	2458	NH1	ARG	321	30.119	68.381	17.997	1.00	65.83
45	ATOM	2459	NH2	ARG	321	28.280	69.750	17.792	1.00	65.76
	ATOM	2460	C	ARG	321	28.765	64.123	24.262	1.00	52.97
	ATOM	2461	O	ARG	321	29.885	64.234	24.758	1.00	53.13
	ATOM	2462	N	GLY	322	28.056	62.996	24.316	1.00	51.39
	ATOM	2463	CA	GLY	322	28.592	61.802	24.950	1.00	49.22
50	ATOM	2464	C	GLY	322	28.198	61.609	26.402	1.00	48.17
	ATOM	2465	O	GLY	322	28.450	60.550	26.986	1.00	48.17
	ATOM	2466	N	ALA	323	27.574	62.627	26.988	1.00	46.66
	ATOM	2467	CA	ALA	323	27.150	62.573	28.385	1.00	44.99
	ATOM	2468	CB	ALA	323	26.462	63.861	28.761	1.00	45.87
55	ATOM	2469	C	ALA	323	26.224	61.403	28.676	1.00	43.43
	ATOM	2470	O	ALA	323	26.514	60.562	29.530	1.00	43.02
	ATOM	2471	N	PHE	324	25.094	61.361	27.981	1.00	41.61
	ATOM	2472	CA	PHE	324	24.147	60.282	28.185	1.00	40.44
	ATOM	2473	CB	PHE	324	22.797	60.631	27.564	1.00	38.94

Figure 4

ATOM	2474	CG	PHE	324	21.644	59.988	28.262	1.00	38.08
ATOM	2475	CD1	PHE	324	21.047	60.613	29.360	1.00	37.48
ATOM	2476	CD2	PHE	324	21.185	58.733	27.860	1.00	36.96
ATOM	2477	CE1	PHE	324	20.010	59.998	30.050	1.00	37.11
ATOM	2478	CE2	PHE	324	20.146	58.105	28.542	1.00	37.79
ATOM	2479	CZ	PHE	324	19.555	58.739	29.643	1.00	37.73
ATOM	2480	C	PHE	324	24.721	59.033	27.525	1.00	40.11
ATOM	2481	O	PHE	324	24.785	58.937	26.289	1.00	40.76
ATOM	2482	N	GLU	325	25.129	58.072	28.350	1.00	39.06
ATOM	2483	CA	GLU	325	25.740	56.851	27.844	1.00	37.85
ATOM	2484	CB	GLU	325	26.846	56.418	28.781	1.00	38.17
ATOM	2485	CG	GLU	325	27.790	57.528	29.085	1.00	40.68
ATOM	2486	CD	GLU	325	28.922	57.075	29.951	1.00	42.47
ATOM	2487	OE1	GLU	325	28.653	56.608	31.086	1.00	44.06
ATOM	2488	OE2	GLU	325	30.080	57.181	29.490	1.00	44.51
ATOM	2489	C	GLU	325	24.799	55.693	27.641	1.00	36.60
ATOM	2490	O	GLU	325	23.903	55.445	28.447	1.00	37.31
ATOM	2491	N	THR	326	25.019	54.968	26.554	1.00	35.30
ATOM	2492	CA	THR	326	24.193	53.816	26.245	1.00	33.37
ATOM	2493	CB	THR	326	24.875	52.921	25.207	1.00	31.58
ATOM	2494	OG1	THR	326	24.934	53.617	23.956	1.00	29.82
ATOM	2495	CG2	THR	326	24.113	51.619	25.041	1.00	29.94
ATOM	2496	C	THR	326	23.951	53.016	27.515	1.00	33.05
ATOM	2497	O	THR	326	22.846	52.528	27.742	1.00	33.99
ATOM	2498	N	ARG	327	24.981	52.902	28.349	1.00	32.29
ATOM	2499	CA	ARG	327	24.859	52.148	29.588	1.00	31.76
ATOM	2500	CB	ARG	327	26.146	52.245	30.417	1.00	33.30
ATOM	2501	CG	ARG	327	26.226	51.162	31.485	1.00	36.71
ATOM	2502	CD	ARG	327	27.596	51.043	32.177	1.00	38.88
ATOM	2503	NE	ARG	327	27.795	52.024	33.249	1.00	40.62
ATOM	2504	CZ	ARG	327	28.274	53.255	33.069	1.00	41.13
ATOM	2505	NH1	ARG	327	28.615	53.670	31.846	1.00	40.49
ATOM	2506	NH2	ARG	327	28.393	54.078	34.113	1.00	40.82
ATOM	2507	C	ARG	327	23.681	52.691	30.387	1.00	30.62
ATOM	2508	O	ARG	327	22.888	51.930	30.940	1.00	29.96
ATOM	2509	N	PHE	328	23.559	54.014	30.425	1.00	29.60
ATOM	2510	CA	PHE	328	22.479	54.660	31.154	1.00	28.70
ATOM	2511	CB	PHE	328	22.632	56.176	31.069	1.00	28.03
ATOM	2512	CG	PHE	328	23.903	56.684	31.686	1.00	27.73
ATOM	2513	CD1	PHE	328	24.337	57.975	31.439	1.00	27.37
ATOM	2514	CD2	PHE	328	24.678	55.857	32.505	1.00	28.92
ATOM	2515	CE1	PHE	328	25.526	58.437	31.992	1.00	28.75
ATOM	2516	CE2	PHE	328	25.871	56.305	33.069	1.00	28.74
ATOM	2517	CZ	PHE	328	26.298	57.599	32.812	1.00	28.68
ATOM	2518	C	PHE	328	21.135	54.226	30.590	1.00	29.06
ATOM	2519	O	PHE	328	20.189	53.953	31.351	1.00	29.59
ATOM	2520	N	VAL	329	21.057	54.154	29.257	1.00	28.40
ATOM	2521	CA	VAL	329	19.830	53.735	28.587	1.00	26.44
ATOM	2522	CB	VAL	329	20.040	53.552	27.059	1.00	25.14
ATOM	2523	CG1	VAL	329	18.737	53.107	26.387	1.00	22.55
ATOM	2524	CG2	VAL	329	20.542	54.841	26.444	1.00	23.05
ATOM	2525	C	VAL	329	19.388	52.399	29.166	1.00	27.98
ATOM	2526	O	VAL	329	18.240	52.239	29.576	1.00	27.88
ATOM	2527	N	SER	330	20.308	51.442	29.219	1.00	28.76
ATOM	2528	CA	SER	330	19.966	50.117	29.718	1.00	30.08
ATOM	2529	CB	SER	330	21.136	49.171	29.534	1.00	30.45
ATOM	2530	OG	SER	330	20.720	47.852	29.822	1.00	31.92
ATOM	2531	C	SER	330	19.534	50.107	31.172	1.00	31.40
ATOM	2532	O	SER	330	18.690	49.298	31.577	1.00	31.74

Figure 4 47/63

	ATOM	2533	N	GLN	331	20.118	50.993	31.972	1.00	32.45
	ATOM	2534	CA	GLN	331	19.745	51.061	33.381	1.00	33.16
	ATOM	2535	CB	GLN	331	20.668	51.992	34.151	1.00	33.58
	ATOM	2536	CG	GLN	331	22.093	51.540	34.194	1.00	35.83
5	ATOM	2537	CD	GLN	331	22.947	52.534	34.919	1.00	37.72
	ATOM	2538	OE1	GLN	331	22.626	52.927	36.043	1.00	39.62
	ATOM	2539	NE2	GLN	331	24.042	52.958	34.291	1.00	38.98
	ATOM	2540	C	GLN	331	18.327	51.591	33.482	1.00	33.78
	ATOM	2541	O	GLN	331	17.428	50.881	33.938	1.00	34.06
10	ATOM	2542	N	VAL	332	18.129	52.835	33.038	1.00	33.77
	ATOM	2543	CA	VAL	332	16.808	53.457	33.097	1.00	33.65
	ATOM	2544	CB	VAL	332	16.760	54.791	32.282	1.00	32.19
	ATOM	2545	CG1	VAL	332	17.279	54.584	30.905	1.00	33.04
	ATOM	2546	CG2	VAL	332	15.340	55.312	32.215	1.00	31.67
15	ATOM	2547	C	VAL	332	15.695	52.505	32.638	1.00	34.20
	ATOM	2548	O	VAL	332	14.571	52.566	33.139	1.00	34.51
	ATOM	2549	N	GLU	333	16.001	51.607	31.711	1.00	34.30
	ATOM	2550	CA	GLU	333	14.981	50.676	31.258	1.00	34.92
	ATOM	2551	CB	GLU	333	15.210	50.289	29.795	1.00	34.40
20	ATOM	2552	CG	GLU	333	14.893	51.413	28.837	1.00	33.07
	ATOM	2553	CD	GLU	333	14.806	50.956	27.409	1.00	31.80
	ATOM	2554	OE1	GLU	333	13.983	50.060	27.114	1.00	31.65
	ATOM	2555	OE2	GLU	333	15.561	51.504	26.581	1.00	31.72
	ATOM	2556	C	GLU	333	14.949	49.438	32.135	1.00	35.76
25	ATOM	2557	O	GLU	333	14.163	48.520	31.911	1.00	35.73
	ATOM	2558	N	SER	334	15.814	49.419	33.138	1.00	36.91
	ATOM	2559	CA	SER	334	15.876	48.307	34.071	1.00	38.13
	ATOM	2560	CB	SER	334	17.328	47.934	34.346	1.00	39.38
	ATOM	2561	OG	SER	334	17.460	46.524	34.468	1.00	41.52
30	ATOM	2562	C	SER	334	15.201	48.747	35.362	1.00	37.93
	ATOM	2563	O	SER	334	15.053	47.973	36.306	1.00	38.63
	ATOM	2564	N	ASP	335	14.807	50.014	35.385	1.00	38.51
	ATOM	2565	CA	ASP	335	14.133	50.619	36.521	1.00	38.59
	ATOM	2566	CB	ASP	335	13.776	52.061	36.173	1.00	39.10
35	ATOM	2567	CG	ASP	335	13.346	52.864	37.373	1.00	39.89
	ATOM	2568	OD1	ASP	335	12.278	52.547	37.950	1.00	40.30
	ATOM	2569	OD2	ASP	335	14.079	53.816	37.737	1.00	39.90
	ATOM	2570	C	ASP	335	12.876	49.809	36.840	1.00	39.11
	ATOM	2571	O	ASP	335	12.241	49.249	35.945	1.00	39.03
40	ATOM	2572	N	THR	336	12.517	49.768	38.119	1.00	39.68
	ATOM	2573	CA	THR	336	11.372	48.999	38.605	1.00	39.94
	ATOM	2574	CB	THR	336	11.773	48.297	39.896	1.00	39.68
	ATOM	2575	OG1	THR	336	12.901	47.464	39.630	1.00	40.95
	ATOM	2576	CG2	THR	336	10.650	47.452	40.426	1.00	39.84
45	ATOM	2577	C	THR	336	10.043	49.735	38.853	1.00	40.52
	ATOM	2578	O	THR	336	8.984	49.108	38.931	1.00	40.91
	ATOM	2579	N	GLY	337	10.085	51.054	38.970	1.00	40.80
	ATOM	2580	CA	GLY	337	8.870	51.804	39.234	1.00	41.83
	ATOM	2581	C	GLY	337	9.307	52.948	40.112	1.00	42.60
50	ATOM	2582	O	GLY	337	8.990	54.105	39.865	1.00	43.33
	ATOM	2583	N	ASP	338	10.043	52.604	41.156	1.00	43.47
	ATOM	2584	CA	ASP	338	10.606	53.589	42.059	1.00	44.40
	ATOM	2585	CB	ASP	338	11.354	52.868	43.175	1.00	44.83
	ATOM	2586	CG	ASP	338	12.303	51.808	42.637	1.00	45.34
55	ATOM	2587	OD1	ASP	338	11.879	51.032	41.751	1.00	46.12
	ATOM	2588	OD2	ASP	338	13.465	51.742	43.087	1.00	45.59
	ATOM	2589	C	ASP	338	11.597	54.296	41.142	1.00	44.84
	ATOM	2590	O	ASP	338	12.605	53.709	40.756	1.00	45.53
	ATOM	2591	N	ARG	339	11.310	55.533	40.763	1.00	44.81

Figure 4

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	ATOM	2592	CA	ARG	339	12.208	56.256	39.874	1.00	45.11
	ATOM	2593	CB	ARG	339	11.702	57.687	39.654	1.00	45.72
	ATOM	2594	CG	ARG	339	10.466	57.799	38.783	1.00	46.11
	ATOM	2595	CD	ARG	339	9.201	57.413	39.521	1.00	46.99
5	ATOM	2596	NE	ARG	339	8.041	57.492	38.633	1.00	47.58
	ATOM	2597	CZ	ARG	339	6.780	57.326	39.017	1.00	47.30
	ATOM	2598	NH1	ARG	339	6.492	57.068	40.287	1.00	47.38
	ATOM	2599	NH2	ARG	339	5.806	57.413	38.123	1.00	47.44
	ATOM	2600	C	ARG	339	13.637	56.295	40.419	1.00	44.98
10	ATOM	2601	O	ARG	339	14.466	57.084	39.960	1.00	44.83
	ATOM	2602	N	LYS	340	13.922	55.441	41.394	1.00	44.75
	ATOM	2603	CA	LYS	340	15.238	55.394	42.001	1.00	45.05
	ATOM	2604	CB	LYS	340	15.341	54.179	42.917	1.00	46.19
	ATOM	2605	CG	LYS	340	14.358	54.250	44.081	1.00	47.87
15	ATOM	2606	CD	LYS	340	14.598	53.154	45.094	1.00	49.25
	ATOM	2607	CE	LYS	340	13.365	52.949	45.957	1.00	50.44
	ATOM	2608	NZ	LYS	340	13.353	51.589	46.598	1.00	51.78
	ATOM	2609	C	LYS	340	16.398	55.422	41.014	1.00	44.66
	ATOM	2610	O	LYS	340	17.186	56.372	41.026	1.00	44.90
20	ATOM	2611	N	GLN	341	16.509	54.408	40.155	1.00	43.94
	ATOM	2612	CA	GLN	341	17.603	54.362	39.174	1.00	42.93
	ATOM	2613	CB	GLN	341	17.598	53.028	38.435	1.00	45.04
	ATOM	2614	CG	GLN	341	18.035	51.860	39.289	1.00	48.03
	ATOM	2615	CD	GLN	341	18.758	50.801	38.482	1.00	49.69
25	ATOM	2616	OE1	GLN	341	19.731	51.101	37.779	1.00	50.67
	ATOM	2617	NE2	GLN	341	18.297	49.556	38.581	1.00	50.43
	ATOM	2618	C	GLN	341	17.616	55.497	38.146	1.00	40.93
	ATOM	2619	O	GLN	341	18.672	56.057	37.839	1.00	38.85
	ATOM	2620	N	ILE	342	16.449	55.824	37.600	1.00	39.61
30	ATOM	2621	CA	ILE	342	16.364	56.905	36.624	1.00	39.07
	ATOM	2622	CB	ILE	342	14.920	57.110	36.130	1.00	39.24
	ATOM	2623	CG2	ILE	342	14.880	58.226	35.107	1.00	39.19
	ATOM	2624	CG1	ILE	342	14.392	55.817	35.501	1.00	39.87
	ATOM	2625	CD1	ILE	342	12.945	55.902	35.070	1.00	40.76
35	ATOM	2626	C	ILE	342	16.832	58.185	37.301	1.00	38.43
	ATOM	2627	O	ILE	342	17.704	58.892	36.795	1.00	37.48
	ATOM	2628	N	TYR	343	16.240	58.466	38.456	1.00	38.93
	ATOM	2629	CA	TYR	343	16.580	59.647	39.236	1.00	39.71
	ATOM	2630	CB	TYR	343	15.813	59.656	40.567	1.00	40.97
40	ATOM	2631	CG	TYR	343	16.173	60.835	41.448	1.00	42.53
	ATOM	2632	CD1	TYR	343	15.344	61.954	41.521	1.00	43.30
	ATOM	2633	CE1	TYR	343	15.730	63.092	42.228	1.00	44.58
	ATOM	2634	CD2	TYR	343	17.397	60.880	42.119	1.00	43.04
	ATOM	2635	CE2	TYR	343	17.791	62.014	42.826	1.00	43.55
45	ATOM	2636	CZ	TYR	343	16.958	63.117	42.872	1.00	44.31
	ATOM	2637	OH	TYR	343	17.369	64.260	43.523	1.00	45.74
	ATOM	2638	C	TYR	343	18.070	59.635	39.532	1.00	39.93
	ATOM	2639	O	TYR	343	18.789	60.598	39.262	1.00	40.28
	ATOM	2640	N	ASN	344	18.525	58.529	40.098	1.00	40.14
50	ATOM	2641	CA	ASN	344	19.924	58.371	40.460	1.00	40.97
	ATOM	2642	CB	ASN	344	20.146	56.958	40.989	1.00	42.94
	ATOM	2643	CG	ASN	344	21.287	56.880	41.977	1.00	44.68
	ATOM	2644	OD1	ASN	344	22.448	57.137	41.628	1.00	46.05
	ATOM	2645	ND2	ASN	344	20.965	56.531	43.225	1.00	44.93
55	ATOM	2646	C	ASN	344	20.869	58.649	39.292	1.00	40.46
	ATOM	2647	O	ASN	344	21.946	59.208	39.483	1.00	40.33
	ATOM	2648	N	ILE	345	20.460	58.262	38.085	1.00	40.50
	ATOM	2649	CA	ILE	345	21.280	58.467	36.890	1.00	39.89
	ATOM	2650	CB	ILE	345	20.803	57.555	35.720	1.00	39.76

Figure 4

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	ATOM	2651	CG2	ILE	345	21.597	57.849	34.448	1.00	38.62
	ATOM	2652	CG1	ILE	345	20.966	56.090	36.114	1.00	38.74
	ATOM	2653	CD1	ILE	345	20.201	55.151	35.242	1.00	38.61
	ATOM	2654	C	ILE	345	21.247	59.924	36.434	1.00	39.80
5	ATOM	2655	O	ILE	345	22.281	60.490	36.074	1.00	39.67
	ATOM	2656	N	LEU	346	20.062	60.529	36.449	1.00	39.59
	ATOM	2657	CA	LEU	346	19.912	61.923	36.029	1.00	39.58
	ATOM	2658	CB	LEU	346	18.434	62.255	35.818	1.00	37.79
	ATOM	2659	CG	LEU	346	17.809	61.528	34.625	1.00	36.58
10	ATOM	2660	CD1	LEU	346	16.277	61.599	34.684	1.00	35.18
	ATOM	2661	CD2	LEU	346	18.363	62.145	33.337	1.00	35.05
	ATOM	2662	C	LEU	346	20.519	62.892	37.034	1.00	40.82
	ATOM	2663	O	LEU	346	21.177	63.857	36.654	1.00	41.02
	ATOM	2664	N	SER	347	20.298	62.646	38.322	1.00	42.34
15	ATOM	2665	CA	SER	347	20.859	63.530	39.339	1.00	43.44
	ATOM	2666	CB	SER	347	20.491	63.042	40.745	1.00	43.90
	ATOM	2667	OG	SER	347	20.665	61.639	40.868	1.00	45.32
	ATOM	2668	C	SER	347	22.368	63.556	39.156	1.00	43.44
	ATOM	2669	O	SER	347	22.974	64.624	39.051	1.00	44.11
20	ATOM	2670	N	THR	348	22.969	62.374	39.096	1.00	43.10
	ATOM	2671	CA	THR	348	24.407	62.285	38.909	1.00	42.97
	ATOM	2672	CB	THR	348	24.853	60.830	38.700	1.00	42.31
	ATOM	2673	OG1	THR	348	24.666	60.096	39.918	1.00	42.08
	ATOM	2674	CG2	THR	348	26.322	60.780	38.282	1.00	40.85
25	ATOM	2675	C	THR	348	24.798	63.093	37.683	1.00	43.25
	ATOM	2676	O	THR	348	25.796	63.813	37.680	1.00	43.52
	ATOM	2677	N	LEU	349	23.990	62.982	36.640	1.00	43.57
	ATOM	2678	CA	LEU	349	24.271	63.697	35.412	1.00	44.17
	ATOM	2679	CB	LEU	349	23.343	63.180	34.311	1.00	44.43
30	ATOM	2680	CG	LEU	349	23.787	63.204	32.847	1.00	44.86
	ATOM	2681	CD1	LEU	349	25.198	62.658	32.688	1.00	44.59
	ATOM	2682	CD2	LEU	349	22.790	62.375	32.046	1.00	44.64
	ATOM	2683	C	LEU	349	24.102	65.201	35.638	1.00	44.32
	ATOM	2684	O	LEU	349	24.317	66.003	34.726	1.00	45.33
35	ATOM	2685	N	GLY	350	23.722	65.574	36.862	1.00	43.94
	ATOM	2686	CA	GLY	350	23.559	66.981	37.210	1.00	43.15
	ATOM	2687	C	GLY	350	22.167	67.570	37.038	1.00	42.49
	ATOM	2688	O	GLY	350	22.024	68.752	36.703	1.00	41.70
	ATOM	2689	N	LEU	351	21.143	66.758	37.288	1.00	41.97
40	ATOM	2690	CA	LEU	351	19.758	67.197	37.132	1.00	41.45
	ATOM	2691	CB	LEU	351	19.194	66.676	35.812	1.00	40.99
	ATOM	2692	CG	LEU	351	19.875	67.115	34.522	1.00	40.66
	ATOM	2693	CD1	LEU	351	19.516	66.144	33.416	1.00	41.63
	ATOM	2694	CD2	LEU	351	19.453	68.533	34.172	1.00	40.77
45	ATOM	2695	C	LEU	351	18.858	66.718	38.262	1.00	41.15
	ATOM	2696	O	LEU	351	19.170	65.760	38.973	1.00	40.88
	ATOM	2697	N	ARG	352	17.720	67.379	38.410	1.00	41.10
	ATOM	2698	CA	ARG	352	16.782	67.007	39.457	1.00	41.25
	ATOM	2699	CB	ARG	352	16.614	68.173	40.431	1.00	42.65
50	ATOM	2700	CG	ARG	352	17.929	68.581	41.070	1.00	43.68
	ATOM	2701	CD	ARG	352	18.504	67.421	41.851	1.00	45.59
	ATOM	2702	NE	ARG	352	19.960	67.478	41.917	1.00	47.73
	ATOM	2703	CZ	ARG	352	20.715	66.567	42.521	1.00	48.77
	ATOM	2704	NH1	ARG	352	20.143	65.524	43.119	1.00	49.05
55	ATOM	2705	NH2	ARG	352	22.038	66.700	42.519	1.00	49.14
	ATOM	2706	C	ARG	352	15.458	66.621	38.827	1.00	39.59
	ATOM	2707	O	ARG	352	14.512	67.399	38.793	1.00	40.34
	ATOM	2708	N	PRO	353	15.378	65.388	38.324	1.00	38.06
	ATOM	2709	CD	PRO	353	16.325	64.285	38.555	1.00	37.28

Figure 4

	ATOM	2710	CA	PRO	353	14.159	64.901	37.683	1.00	37.45
	ATOM	2711	CB	PRO	353	14.595	63.552	37.134	1.00	37.27
	ATOM	2712	CG	PRO	353	15.491	63.064	38.232	1.00	36.92
	ATOM	2713	C	PRO	353	12.998	64.763	38.650	1.00	36.35
5	ATOM	2714	O	PRO	353	13.180	64.360	39.791	1.00	36.28
	ATOM	2715	N	SER	354	11.805	65.110	38.194	1.00	35.82
	ATOM	2716	CA	SER	354	10.625	64.951	39.028	1.00	36.40
	ATOM	2717	CB	SER	354	9.570	66.010	38.698	1.00	35.94
	ATOM	2718	OG	SER	354	8.944	65.725	37.459	1.00	35.63
10	ATOM	2719	C	SER	354	10.091	63.570	38.653	1.00	36.41
	ATOM	2720	O	SER	354	10.592	62.948	37.716	1.00	37.42
	ATOM	2721	N	THR	355	9.087	63.091	39.375	1.00	36.02
	ATOM	2722	CA	THR	355	8.493	61.790	39.099	1.00	35.68
	ATOM	2723	CB	THR	355	7.200	61.615	39.923	1.00	36.38
15	ATOM	2724	OG1	THR	355	7.525	61.645	41.316	1.00	37.75
	ATOM	2725	CG2	THR	355	6.510	60.293	39.598	1.00	36.44
	ATOM	2726	C	THR	355	8.161	61.633	37.609	1.00	35.80
	ATOM	2727	O	THR	355	8.319	60.548	37.029	1.00	34.73
	ATOM	2728	N	THR	356	7.698	62.720	36.994	1.00	35.28
20	ATOM	2729	CA	THR	356	7.336	62.690	35.586	1.00	35.39
	ATOM	2730	CB	THR	356	6.287	63.774	35.263	1.00	35.59
	ATOM	2731	OG1	THR	356	6.651	64.990	35.925	1.00	35.39
	ATOM	2732	CG2	THR	356	4.892	63.331	35.719	1.00	34.33
	ATOM	2733	C	THR	356	8.542	62.848	34.662	1.00	35.30
25	ATOM	2734	O	THR	356	8.560	62.285	33.559	1.00	34.91
	ATOM	2735	N	ASP	357	9.537	63.624	35.089	1.00	35.07
	ATOM	2736	CA	ASP	357	10.740	63.782	34.277	1.00	35.80
	ATOM	2737	CB	ASP	357	11.804	64.598	35.012	1.00	36.76
	ATOM	2738	CG	ASP	357	11.451	66.077	35.116	1.00	38.19
30	ATOM	2739	OD1	ASP	357	11.475	66.778	34.071	1.00	37.60
	ATOM	2740	OD2	ASP	357	11.158	66.538	36.249	1.00	38.76
	ATOM	2741	C	ASP	357	11.277	62.373	34.039	1.00	35.97
	ATOM	2742	O	ASP	357	11.460	61.942	32.901	1.00	36.94
	ATOM	2743	N	CYS	358	11.498	61.649	35.131	1.00	35.67
35	ATOM	2744	CA	CYS	358	12.013	60.293	35.057	1.00	35.44
	ATOM	2745	CB	CYS	358	12.051	59.658	36.447	1.00	35.93
	ATOM	2746	SG	CYS	358	13.247	60.410	37.575	1.00	35.81
	ATOM	2747	C	CYS	358	11.177	59.433	34.138	1.00	34.88
	ATOM	2748	O	CYS	358	11.711	58.698	33.308	1.00	35.87
40	ATOM	2749	N	ASP	359	9.863	59.517	34.290	1.00	34.10
	ATOM	2750	CA	ASP	359	8.960	58.729	33.464	1.00	33.10
	ATOM	2751	CB	ASP	359	7.519	58.964	33.910	1.00	35.03
	ATOM	2752	CG	ASP	359	7.118	58.058	35.062	1.00	36.65
	ATOM	2753	OD1	ASP	359	7.950	57.850	35.975	1.00	38.15
45	ATOM	2754	OD2	ASP	359	5.969	57.561	35.055	1.00	37.12
	ATOM	2755	C	ASP	359	9.130	59.058	31.985	1.00	31.16
	ATOM	2756	O	ASP	359	9.090	58.170	31.133	1.00	30.01
	ATOM	2757	N	ILE	360	9.325	60.334	31.682	1.00	29.54
	ATOM	2758	CA	ILE	360	9.524	60.741	30.300	1.00	28.61
50	ATOM	2759	CB	ILE	360	9.546	62.273	30.162	1.00	27.75
	ATOM	2760	CG2	ILE	360	10.255	62.668	28.874	1.00	27.01
	ATOM	2761	CG1	ILE	360	8.112	62.818	30.235	1.00	26.18
	ATOM	2762	CD1	ILE	360	8.024	64.322	30.190	1.00	23.23
	ATOM	2763	C	ILE	360	10.857	60.176	29.825	1.00	29.21
55	ATOM	2764	O	ILE	360	10.919	59.480	28.805	1.00	29.88
	ATOM	2765	N	VAL	361	11.923	60.466	30.569	1.00	28.39
	ATOM	2766	CA	VAL	361	13.248	59.971	30.219	1.00	28.01
	ATOM	2767	CB	VAL	361	14.258	60.256	31.342	1.00	27.73
	ATOM	2768	CG1	VAL	361	15.575	59.551	31.055	1.00	27.43

Figure 4

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ATOM	2769	CG2	VAL	361	14.492	61.759	31.453	1.00	27.76
ATOM	2770	C	VAL	361	13.245	58.464	29.919	1.00	27.74
ATOM	2771	O	VAL	361	14.055	57.982	29.107	1.00	27.40
ATOM	2772	N	ARG	362	12.341	57.719	30.556	1.00	27.72
ATOM	2773	CA	ARG	362	12.277	56.275	30.325	1.00	27.95
ATOM	2774	CB	ARG	362	11.523	55.571	31.455	1.00	29.48
ATOM	2775	CG	ARG	362	11.137	54.147	31.101	1.00	31.97
ATOM	2776	CD	ARG	362	10.900	53.266	32.308	1.00	33.93
ATOM	2777	NE	ARG	362	10.930	51.859	31.893	1.00	37.37
ATOM	2778	CZ	ARG	362	10.938	50.817	32.725	1.00	37.52
ATOM	2779	NH1	ARG	362	10.920	51.010	34.043	1.00	38.72
ATOM	2780	NH2	ARG	362	10.960	49.582	32.230	1.00	36.06
ATOM	2781	C	ARG	362	11.614	55.959	28.994	1.00	27.88
ATOM	2782	O	ARG	362	12.016	55.032	28.289	1.00	29.02
ATOM	2783	N	ARG	363	10.586	56.728	28.660	1.00	27.31
ATOM	2784	CA	ARG	363	9.866	56.564	27.400	1.00	25.77
ATOM	2785	CB	ARG	363	8.641	57.486	27.374	1.00	26.51
ATOM	2786	CG	ARG	363	7.530	57.084	28.318	1.00	26.30
ATOM	2787	CD	ARG	363	6.730	55.929	27.739	1.00	28.36
ATOM	2788	NE	ARG	363	6.259	56.216	26.380	1.00	30.91
ATOM	2789	CZ	ARG	363	6.872	55.826	25.260	1.00	31.55
ATOM	2790	NH1	ARG	363	7.992	55.112	25.315	1.00	33.18
ATOM	2791	NH2	ARG	363	6.370	56.158	24.077	1.00	32.30
ATOM	2792	C	ARG	363	10.817	56.949	26.272	1.00	24.71
ATOM	2793	O	ARG	363	10.748	56.392	25.175	1.00	24.40
ATOM	2794	N	ALA	364	11.706	57.905	26.540	1.00	23.90
ATOM	2795	CA	ALA	364	12.653	58.339	25.507	1.00	24.48
ATOM	2796	CB	ALA	364	13.463	59.545	25.969	1.00	23.15
ATOM	2797	C	ALA	364	13.571	57.176	25.226	1.00	25.01
ATOM	2798	O	ALA	364	13.854	56.872	24.069	1.00	26.22
ATOM	2799	N	CYS	365	14.023	56.518	26.290	1.00	25.03
ATOM	2800	CA	CYS	365	14.902	55.370	26.157	1.00	24.77
ATOM	2801	CB	CYS	365	15.450	54.970	27.528	1.00	23.03
ATOM	2802	SG	CYS	365	16.728	56.114	28.173	1.00	21.60
ATOM	2803	C	CYS	365	14.140	54.206	25.514	1.00	26.44
ATOM	2804	O	CYS	365	14.661	53.535	24.617	1.00	27.49
ATOM	2805	N	GLU	366	12.906	53.956	25.944	1.00	26.87
ATOM	2806	CA	GLU	366	12.145	52.859	25.342	1.00	27.98
ATOM	2807	CB	GLU	366	10.757	52.743	25.988	1.00	28.74
ATOM	2808	CG	GLU	366	10.785	52.431	27.490	1.00	30.75
ATOM	2809	CD	GLU	366	9.427	51.981	28.041	1.00	32.09
ATOM	2810	OE1	GLU	366	8.444	52.757	27.970	1.00	32.39
ATOM	2811	OE2	GLU	366	9.342	50.841	28.547	1.00	33.30
ATOM	2812	C	GLU	366	12.005	53.056	23.815	1.00	28.15
ATOM	2813	O	GLU	366	12.117	52.104	23.029	1.00	27.63
ATOM	2814	N	SER	367	11.776	54.304	23.407	1.00	28.42
ATOM	2815	CA	SER	367	11.612	54.650	21.993	1.00	27.23
ATOM	2816	CB	SER	367	11.368	56.156	21.833	1.00	27.45
ATOM	2817	OG	SER	367	10.161	56.552	22.447	1.00	27.44
ATOM	2818	C	SER	367	12.824	54.276	21.165	1.00	26.52
ATOM	2819	O	SER	367	12.724	53.567	20.162	1.00	27.99
ATOM	2820	N	VAL	368	13.977	54.773	21.581	1.00	24.30
ATOM	2821	CA	VAL	368	15.194	54.499	20.849	1.00	22.45
ATOM	2822	CB	VAL	368	16.324	55.395	21.375	1.00	20.96
ATOM	2823	CG1	VAL	368	17.623	55.075	20.682	1.00	18.44
ATOM	2824	CG2	VAL	368	15.928	56.843	21.190	1.00	18.99
ATOM	2825	C	VAL	368	15.605	53.019	20.888	1.00	23.13
ATOM	2826	O	VAL	368	15.850	52.420	19.832	1.00	23.88
ATOM	2827	N	SER	369	15.660	52.405	22.071	1.00	22.54

Figure 4

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	ATOM	2828	CA	SER	369	16.071	51.003	22.106	1.00	21.93
	ATOM	2829	CB	SER	369	16.248	50.476	23.542	1.00	23.39
	ATOM	2830	OG	SER	369	15.011	50.251	24.197	1.00	25.91
	ATOM	2831	C	SER	369	15.109	50.112	21.348	1.00	20.54
5	ATOM	2832	O	SER	369	15.526	49.063	20.850	1.00	20.31
	ATOM	2833	N	THR	370	13.832	50.499	21.259	1.00	18.40
	ATOM	2834	CA	THR	370	12.878	49.682	20.496	1.00	17.32
	ATOM	2835	CB	THR	370	11.400	49.976	20.859	1.00	16.46
	ATOM	2836	OG1	THR	370	11.053	49.298	22.073	1.00	15.81
10	ATOM	2837	CG2	THR	370	10.473	49.487	19.774	1.00	14.39
	ATOM	2838	C	THR	370	13.076	49.936	19.001	1.00	17.03
	ATOM	2839	O	THR	370	12.977	49.008	18.186	1.00	17.38
	ATOM	2840	N	ARG	371	13.358	51.177	18.617	1.00	16.71
	ATOM	2841	CA	ARG	371	13.562	51.423	17.201	1.00	16.54
15	ATOM	2842	CB	ARG	371	13.810	52.905	16.882	1.00	17.42
	ATOM	2843	CG	ARG	371	14.013	53.123	15.374	1.00	17.76
	ATOM	2844	CD	ARG	371	14.283	54.559	14.943	1.00	17.40
	ATOM	2845	NE	ARG	371	15.567	55.076	15.412	1.00	18.85
	ATOM	2846	CZ	ARG	371	16.159	56.154	14.896	1.00	18.99
20	ATOM	2847	NH1	ARG	371	15.583	56.810	13.892	1.00	17.43
	ATOM	2848	NH2	ARG	371	17.303	56.605	15.406	1.00	19.19
	ATOM	2849	C	ARG	371	14.763	50.607	16.759	1.00	15.91
	ATOM	2850	O	ARG	371	14.689	49.929	15.748	1.00	17.14
	ATOM	2851	N	ALA	372	15.856	50.644	17.519	1.00	15.40
25	ATOM	2852	CA	ALA	372	17.061	49.883	17.148	1.00	16.23
	ATOM	2853	CB	ALA	372	18.152	50.046	18.197	1.00	15.66
	ATOM	2854	C	ALA	372	16.775	48.407	16.957	1.00	16.83
	ATOM	2855	O	ALA	372	17.125	47.838	15.923	1.00	18.06
	ATOM	2856	N	ALA	373	16.149	47.790	17.955	1.00	16.86
30	ATOM	2857	CA	ALA	373	15.817	46.367	17.912	1.00	17.10
	ATOM	2858	CB	ALA	373	15.027	45.976	19.156	1.00	16.66
	ATOM	2859	C	ALA	373	15.024	46.018	16.665	1.00	18.79
	ATOM	2860	O	ALA	373	15.301	45.004	16.018	1.00	20.02
	ATOM	2861	N	HIS	374	14.037	46.841	16.316	1.00	19.22
35	ATOM	2862	CA	HIS	374	13.243	46.560	15.122	1.00	20.89
	ATOM	2863	CB	HIS	374	12.025	47.489	15.052	1.00	20.98
	ATOM	2864	CG	HIS	374	10.948	47.131	16.029	1.00	19.79
	ATOM	2865	CD2	HIS	374	10.813	46.065	16.855	1.00	19.53
	ATOM	2866	ND1	HIS	374	9.833	47.914	16.229	1.00	19.92
40	ATOM	2867	CE1	HIS	374	9.057	47.347	17.137	1.00	18.78
	ATOM	2868	NE2	HIS	374	9.629	46.223	17.532	1.00	18.61
	ATOM	2869	C	HIS	374	14.075	46.696	13.866	1.00	21.57
	ATOM	2870	O	HIS	374	14.136	45.789	13.058	1.00	21.42
	ATOM	2871	N	MSE	375	14.722	47.835	13.698	1.00	24.00
45	ATOM	2872	CA	MSE	375	15.561	48.027	12.528	1.00	26.05
	ATOM	2873	CB	MSE	375	16.390	49.311	12.666	1.00	28.31
	ATOM	2874	CG	MSE	375	15.671	50.558	12.197	1.00	31.46
	ATOM	2875	SE	MSE	375	15.246	50.448	10.400	1.00	41.26
	ATOM	2876	CE	MSE	375	16.340	51.745	9.680	1.00	36.51
50	ATOM	2877	C	MSE	375	16.476	46.810	12.390	1.00	25.84
	ATOM	2878	O	MSE	375	16.501	46.159	11.351	1.00	26.84
	ATOM	2879	N	CYS	376	17.200	46.489	13.455	1.00	25.61
	ATOM	2880	CA	CYS	376	18.107	45.349	13.436	1.00	25.11
	ATOM	2881	CB	CYS	376	18.693	45.117	14.831	1.00	26.04
55	ATOM	2882	SG	CYS	376	20.038	43.879	14.876	1.00	27.98
	ATOM	2883	C	CYS	376	17.445	44.058	12.931	1.00	24.01
	ATOM	2884	O	CYS	376	18.015	43.369	12.078	1.00	24.35
	ATOM	2885	N	SER	377	16.251	43.741	13.443	1.00	22.14
	ATOM	2886	CA	SER	377	15.519	42.531	13.038	1.00	20.58

Figure 4

	ATOM	2887	CB	SER	377	14.203	42.399	13.811	1.00	20.36
	ATOM	2888	OG	SER	377	13.233	43.325	13.338	1.00	20.95
	ATOM	2889	C	SER	377	15.210	42.535	11.542	1.00	20.00
	ATOM	2890	O	SER	377	15.154	41.484	10.900	1.00	19.23
5	ATOM	2891	N	ALA	378	14.995	43.715	10.980	1.00	19.64
	ATOM	2892	CA	ALA	378	14.723	43.787	9.549	1.00	19.32
	ATOM	2893	CB	ALA	378	14.521	45.243	9.119	1.00	18.02
	ATOM	2894	C	ALA	378	15.958	43.186	8.874	1.00	19.40
	ATOM	2895	O	ALA	378	15.860	42.230	8.093	1.00	18.55
10	ATOM	2896	N	GLY	379	17.123	43.740	9.222	1.00	20.18
	ATOM	2897	CA	GLY	379	18.381	43.271	8.669	1.00	20.06
	ATOM	2898	C	GLY	379	18.547	41.762	8.734	1.00	19.52
	ATOM	2899	O	GLY	379	18.754	41.113	7.704	1.00	20.07
	ATOM	2900	N	LEU	380	18.442	41.201	9.936	1.00	18.61
15	ATOM	2901	CA	LEU	380	18.596	39.763	10.110	1.00	18.74
	ATOM	2902	CB	LEU	380	18.489	39.371	11.579	1.00	18.49
	ATOM	2903	CG	LEU	380	18.774	37.881	11.816	1.00	17.82
	ATOM	2904	CD1	LEU	380	20.215	37.586	11.383	1.00	16.94
	ATOM	2905	CD2	LEU	380	18.557	37.512	13.285	1.00	16.34
20	ATOM	2906	C	LEU	380	17.580	38.938	9.341	1.00	19.56
	ATOM	2907	O	LEU	380	17.895	37.833	8.892	1.00	20.67
	ATOM	2908	N	ALA	381	16.354	39.447	9.211	1.00	19.83
	ATOM	2909	CA	ALA	381	15.311	38.713	8.496	1.00	20.17
	ATOM	2910	CB	ALA	381	13.961	39.327	8.759	1.00	19.87
25	ATOM	2911	C	ALA	381	15.638	38.746	7.009	1.00	21.06
	ATOM	2912	O	ALA	381	15.421	37.773	6.269	1.00	21.05
	ATOM	2913	N	GLY	382	16.174	39.874	6.567	1.00	21.33
	ATOM	2914	CA	GLY	382	16.561	39.965	5.175	1.00	22.63
	ATOM	2915	C	GLY	382	17.670	38.954	4.903	1.00	23.10
30	ATOM	2916	O	GLY	382	17.708	38.319	3.832	1.00	23.74
	ATOM	2917	N	VAL	383	18.579	38.778	5.859	1.00	21.83
	ATOM	2918	CA	VAL	383	19.642	37.828	5.615	1.00	22.47
	ATOM	2919	CB	VAL	383	20.786	37.967	6.643	1.00	22.80
	ATOM	2920	CG1	VAL	383	21.737	36.777	6.525	1.00	21.04
35	ATOM	2921	CG2	VAL	383	21.562	39.298	6.396	1.00	21.85
	ATOM	2922	C	VAL	383	19.075	36.423	5.639	1.00	22.92
	ATOM	2923	O	VAL	383	19.199	35.681	4.675	1.00	23.65
	ATOM	2924	N	ILE	384	18.414	36.061	6.724	1.00	23.52
	ATOM	2925	CA	ILE	384	17.853	34.721	6.835	1.00	24.64
40	ATOM	2926	CB	ILE	384	17.124	34.551	8.179	1.00	24.17
	ATOM	2927	CG2	ILE	384	16.533	33.143	8.283	1.00	22.50
	ATOM	2928	CG1	ILE	384	18.112	34.810	9.318	1.00	23.69
	ATOM	2929	CD1	ILE	384	17.476	34.861	10.661	1.00	24.39
	ATOM	2930	C	ILE	384	16.910	34.324	5.691	1.00	26.04
45	ATOM	2931	O	ILE	384	17.029	33.233	5.144	1.00	26.98
	ATOM	2932	N	ASN	385	15.974	35.182	5.310	1.00	26.88
	ATOM	2933	CA	ASN	385	15.097	34.785	4.218	1.00	27.99
	ATOM	2934	CB	ASN	385	13.984	35.819	3.998	1.00	25.92
	ATOM	2935	CG	ASN	385	13.038	35.918	5.174	1.00	23.68
50	ATOM	2936	OD1	ASN	385	12.721	34.921	5.820	1.00	21.60
	ATOM	2937	ND2	ASN	385	12.567	37.128	5.448	1.00	23.03
	ATOM	2938	C	ASN	385	15.888	34.579	2.915	1.00	29.62
	ATOM	2939	O	ASN	385	15.610	33.647	2.143	1.00	29.62
	ATOM	2940	N	ARG	386	16.869	35.440	2.660	1.00	31.30
55	ATOM	2941	CA	ARG	386	17.660	35.301	1.442	1.00	33.07
	ATOM	2942	CB	ARG	386	18.840	36.261	1.446	1.00	32.62
	ATOM	2943	CG	ARG	386	19.697	36.147	0.214	1.00	33.28
	ATOM	2944	CD	ARG	386	20.908	37.059	0.284	1.00	34.52
	ATOM	2945	NE	ARG	386	21.923	36.698	-0.704	1.00	35.29

Figure 4

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	ATOM	2946	CZ	ARG	386	21.812	36.910	-2.014	1.00	36.32
	ATOM	2947	NH1	ARG	386	20.729	37.492	-2.518	1.00	35.95
	ATOM	2948	NH2	ARG	386	22.782	36.525	-2.832	1.00	37.07
	ATOM	2949	C	ARG	386	18.178	33.875	1.362	1.00	34.69
5	ATOM	2950	O	ARG	386	18.077	33.232	0.320	1.00	35.70
	ATOM	2951	N	MSE	387	18.710	33.383	2.480	1.00	35.94
	ATOM	2952	CA	MSE	387	19.250	32.036	2.560	1.00	37.39
	ATOM	2953	CB	MSE	387	19.903	31.828	3.927	1.00	39.78
	ATOM	2954	CG	MSE	387	21.099	32.754	4.186	1.00	42.37
10	ATOM	2955	SE	MSE	387	21.873	32.552	5.859	1.00	49.18
	ATOM	2956	CE	MSE	387	21.738	30.694	6.097	1.00	44.67
	ATOM	2957	C	MSE	387	18.179	30.976	2.311	1.00	38.50
	ATOM	2958	O	MSE	387	18.463	29.927	1.721	1.00	37.80
	ATOM	2959	N	ARG	388	16.954	31.255	2.769	1.00	40.15
15	ATOM	2960	CA	ARG	388	15.808	30.352	2.586	1.00	41.28
	ATOM	2961	CB	ARG	388	14.554	30.941	3.245	1.00	42.50
	ATOM	2962	CG	ARG	388	13.268	30.115	3.069	1.00	42.73
	ATOM	2963	CD	ARG	388	12.266	30.443	4.178	1.00	43.15
	ATOM	2964	NE	ARG	388	10.965	29.787	4.012	1.00	44.47
20	ATOM	2965	CZ	ARG	388	10.049	30.134	3.104	1.00	44.46
	ATOM	2966	NH1	ARG	388	10.283	31.139	2.269	1.00	44.11
	ATOM	2967	NH2	ARG	388	8.895	29.478	3.033	1.00	44.15
	ATOM	2968	C	ARG	388	15.579	30.210	1.094	1.00	41.39
	ATOM	2969	O	ARG	388	15.516	29.104	0.554	1.00	40.76
25	ATOM	2970	N	GLU	389	15.460	31.355	0.439	1.00	41.88
	ATOM	2971	CA	GLU	389	15.275	31.405	-0.997	1.00	43.37
	ATOM	2972	CB	GLU	389	15.211	32.867	-1.448	1.00	45.21
	ATOM	2973	CG	GLU	389	15.227	33.079	-2.957	1.00	48.22
	ATOM	2974	CD	GLU	389	13.894	32.754	-3.632	1.00	50.35
30	ATOM	2975	OE1	GLU	389	13.850	32.799	-4.891	1.00	51.00
	ATOM	2976	OE2	GLU	389	12.900	32.464	-2.912	1.00	50.86
	ATOM	2977	C	GLU	389	16.476	30.713	-1.635	1.00	43.77
	ATOM	2978	O	GLU	389	16.325	29.726	-2.355	1.00	43.53
	ATOM	2979	N	SER	390	17.671	31.227	-1.335	1.00	43.84
35	ATOM	2980	CA	SER	390	18.925	30.697	-1.878	1.00	43.61
	ATOM	2981	CB	SER	390	20.112	31.549	-1.425	1.00	43.41
	ATOM	2982	OG	SER	390	20.229	32.703	-2.241	1.00	43.45
	ATOM	2983	C	SER	390	19.243	29.234	-1.607	1.00	43.62
	ATOM	2984	O	SER	390	20.126	28.671	-2.251	1.00	44.11
40	ATOM	2985	N	ARG	391	18.555	28.614	-0.660	1.00	43.22
	ATOM	2986	CA	ARG	391	18.815	27.213	-0.396	1.00	43.67
	ATOM	2987	CB	ARG	391	19.174	26.994	1.078	1.00	42.72
	ATOM	2988	CG	ARG	391	20.440	27.699	1.512	1.00	41.51
	ATOM	2989	CD	ARG	391	20.907	27.245	2.892	1.00	39.51
45	ATOM	2990	NE	ARG	391	22.183	27.864	3.231	1.00	37.99
	ATOM	2991	CZ	ARG	391	22.940	27.512	4.266	1.00	37.81
	ATOM	2992	NH1	ARG	391	22.545	26.540	5.070	1.00	36.05
	ATOM	2993	NH2	ARG	391	24.105	28.121	4.482	1.00	37.12
	ATOM	2994	C	ARG	391	17.578	26.404	-0.756	1.00	44.95
50	ATOM	2995	O	ARG	391	17.458	25.241	-0.372	1.00	45.05
	ATOM	2996	N	SER	392	16.666	27.023	-1.502	1.00	46.71
	ATOM	2997	CA	SER	392	15.420	26.367	-1.895	1.00	48.25
	ATOM	2998	CB	SER	392	15.631	25.468	-3.121	1.00	48.10
	ATOM	2999	OG	SER	392	15.610	26.216	-4.326	1.00	48.60
55	ATOM	3000	C	SER	392	14.880	25.536	-0.737	1.00	49.61
	ATOM	3001	O	SER	392	14.601	24.344	-0.882	1.00	49.37
	ATOM	3002	N	GLU	393	14.749	26.175	0.420	1.00	51.58
	ATOM	3003	CA	GLU	393	14.237	25.510	1.617	1.00	53.54
	ATOM	3004	CB	GLU	393	15.085	25.897	2.842	1.00	54.33

Figure 4

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ATOM	3005	CG	GLU	393	16.586	25.655	2.701	1.00	54.92
ATOM	3006	CD	GLU	393	17.057	24.420	3.450	1.00	55.87
ATOM	3007	OE1	GLU	393	16.845	24.347	4.683	1.00	55.29
ATOM	3008	OE2	GLU	393	17.646	23.523	2.806	1.00	56.69
ATOM	3009	C	GLU	393	12.793	25.961	1.838	1.00	54.20
ATOM	3010	O	GLU	393	12.482	27.151	1.693	1.00	53.70
ATOM	3011	N	ASP	394	11.907	25.026	2.173	1.00	55.42
ATOM	3012	CA	ASP	394	10.519	25.404	2.419	1.00	56.88
ATOM	3013	CB	ASP	394	9.585	24.194	2.400	1.00	58.69
ATOM	3014	CG	ASP	394	8.111	24.602	2.415	1.00	61.23
ATOM	3015	OD1	ASP	394	7.691	25.298	3.376	1.00	62.29
ATOM	3016	OD2	ASP	394	7.374	24.237	1.466	1.00	62.03
ATOM	3017	C	ASP	394	10.489	26.041	3.795	1.00	56.57
ATOM	3018	O	ASP	394	10.023	27.164	3.959	1.00	56.22
ATOM	3019	N	VAL	395	10.994	25.298	4.773	1.00	56.79
ATOM	3020	CA	VAL	395	11.086	25.756	6.153	1.00	57.23
ATOM	3021	CB	VAL	395	10.166	24.949	7.093	1.00	57.72
ATOM	3022	CG1	VAL	395	10.444	25.320	8.548	1.00	57.64
ATOM	3023	CG2	VAL	395	8.708	25.221	6.749	1.00	58.46
ATOM	3024	C	VAL	395	12.534	25.538	6.575	1.00	57.01
ATOM	3025	O	VAL	395	12.968	24.407	6.793	1.00	56.90
ATOM	3026	N	MSE	396	13.280	26.626	6.690	1.00	56.80
ATOM	3027	CA	MSE	396	14.682	26.536	7.058	1.00	56.12
ATOM	3028	CB	MSE	396	15.463	27.645	6.375	1.00	57.66
ATOM	3029	CG	MSE	396	16.932	27.623	6.690	1.00	60.51
ATOM	3030	SE	MSE	396	17.716	29.077	6.002	1.00	65.26
ATOM	3031	CE	MSE	396	17.988	28.564	4.293	1.00	64.74
ATOM	3032	C	MSE	396	14.964	26.600	8.545	1.00	54.59
ATOM	3033	O	MSE	396	14.487	27.491	9.245	1.00	54.08
ATOM	3034	N	ARG	397	15.740	25.637	9.025	1.00	53.05
ATOM	3035	CA	ARG	397	16.134	25.613	10.426	1.00	51.13
ATOM	3036	CB	ARG	397	16.226	24.181	10.951	1.00	52.77
ATOM	3037	CG	ARG	397	14.888	23.520	11.244	1.00	55.36
ATOM	3038	CD	ARG	397	15.132	22.079	11.671	1.00	58.69
ATOM	3039	NE	ARG	397	13.985	21.448	12.326	1.00	61.28
ATOM	3040	CZ	ARG	397	14.056	20.294	12.990	1.00	62.10
ATOM	3041	NH1	ARG	397	15.215	19.651	13.078	1.00	62.57
ATOM	3042	NH2	ARG	397	12.978	19.793	13.583	1.00	62.49
ATOM	3043	C	ARG	397	17.509	26.252	10.397	1.00	48.33
ATOM	3044	O	ARG	397	18.273	26.029	9.466	1.00	47.77
ATOM	3045	N	ILE	398	17.825	27.064	11.395	1.00	45.82
ATOM	3046	CA	ILE	398	19.120	27.721	11.396	1.00	43.01
ATOM	3047	CB	ILE	398	19.202	28.791	10.293	1.00	43.25
ATOM	3048	CG2	ILE	398	18.161	29.864	10.532	1.00	43.18
ATOM	3049	CG1	ILE	398	20.594	29.417	10.279	1.00	43.75
ATOM	3050	CD1	ILE	398	20.768	30.466	9.206	1.00	44.64
ATOM	3051	C	ILE	398	19.441	28.381	12.717	1.00	40.64
ATOM	3052	O	ILE	398	18.557	28.890	13.404	1.00	40.10
ATOM	3053	N	THR	399	20.722	28.360	13.060	1.00	37.78
ATOM	3054	CA	THR	399	21.185	28.954	14.290	1.00	35.36
ATOM	3055	CB	THR	399	22.052	27.988	15.079	1.00	35.02
ATOM	3056	OG1	THR	399	21.280	26.832	15.425	1.00	34.92
ATOM	3057	CG2	THR	399	22.570	28.666	16.345	1.00	34.73
ATOM	3058	C	THR	399	22.001	30.197	13.994	1.00	34.71
ATOM	3059	O	THR	399	22.736	30.254	13.005	1.00	35.10
ATOM	3060	N	VAL	400	21.858	31.184	14.871	1.00	32.96
ATOM	3061	CA	VAL	400	22.539	32.457	14.759	1.00	31.07
ATOM	3062	CB	VAL	400	21.514	33.593	14.592	1.00	31.21
ATOM	3063	CG1	VAL	400	22.211	34.934	14.415	1.00	31.76

Figure 4

	ATOM	3064	CG2	VAL	400	20.628	33.298	13.405	1.00	31.47
	ATOM	3065	C	VAL	400	23.336	32.685	16.039	1.00	30.19
	ATOM	3066	O	VAL	400	22.779	32.640	17.144	1.00	30.96
	ATOM	3067	N	GLY	401	24.641	32.905	15.888	1.00	28.35
5	ATOM	3068	CA	GLY	401	25.482	33.150	17.041	1.00	24.47
	ATOM	3069	C	GLY	401	25.487	34.641	17.235	1.00	23.04
	ATOM	3070	O	GLY	401	25.595	35.388	16.260	1.00	20.38
	ATOM	3071	N	VAL	402	25.367	35.086	18.482	1.00	23.36
	ATOM	3072	CA	VAL	402	25.338	36.514	18.751	1.00	23.38
10	ATOM	3073	CB	VAL	402	23.927	36.960	19.124	1.00	22.79
	ATOM	3074	CG1	VAL	402	23.790	38.458	18.909	1.00	22.85
	ATOM	3075	CG2	VAL	402	22.895	36.176	18.320	1.00	22.42
	ATOM	3076	C	VAL	402	26.252	36.899	19.893	1.00	24.25
	ATOM	3077	O	VAL	402	26.484	36.098	20.794	1.00	25.20
15	ATOM	3078	N	ASP	403	26.770	38.124	19.848	1.00	24.83
	ATOM	3079	CA	ASP	403	27.637	38.649	20.894	1.00	27.11
	ATOM	3080	CB	ASP	403	29.078	38.212	20.691	1.00	30.98
	ATOM	3081	CG	ASP	403	30.003	38.739	21.787	1.00	34.48
	ATOM	3082	OD1	ASP	403	29.887	39.938	22.122	1.00	36.02
20	ATOM	3083	OD2	ASP	403	30.842	37.960	22.311	1.00	36.05
	ATOM	3084	C	ASP	403	27.562	40.154	20.763	1.00	27.24
	ATOM	3085	O	ASP	403	27.550	40.667	19.645	1.00	29.15
	ATOM	3086	N	GLY	404	27.519	40.863	21.888	1.00	26.60
	ATOM	3087	CA	GLY	404	27.410	42.316	21.863	1.00	26.50
25	ATOM	3088	C	GLY	404	26.750	42.829	23.137	1.00	27.10
	ATOM	3089	O	GLY	404	25.810	42.193	23.665	1.00	26.90
	ATOM	3090	N	SER	405	27.209	43.972	23.644	1.00	26.72
	ATOM	3091	CA	SER	405	26.638	44.496	24.887	1.00	27.96
	ATOM	3092	CB	SER	405	27.409	45.722	25.371	1.00	28.04
30	ATOM	3093	OG	SER	405	27.164	46.828	24.521	1.00	30.53
	ATOM	3094	C	SER	405	25.168	44.857	24.738	1.00	28.25
	ATOM	3095	O	SER	405	24.341	44.473	25.573	1.00	27.96
	ATOM	3096	N	VAL	406	24.844	45.591	23.675	1.00	27.79
	ATOM	3097	CA	VAL	406	23.465	45.992	23.445	1.00	28.13
35	ATOM	3098	CB	VAL	406	23.281	46.667	22.074	1.00	28.02
	ATOM	3099	CG1	VAL	406	21.814	47.063	21.908	1.00	27.91
	ATOM	3100	CG2	VAL	406	24.197	47.877	21.940	1.00	26.07
	ATOM	3101	C	VAL	406	22.535	44.789	23.488	1.00	28.35
	ATOM	3102	O	VAL	406	21.484	44.826	24.120	1.00	28.48
40	ATOM	3103	N	TYR	407	22.934	43.718	22.811	1.00	28.72
	ATOM	3104	CA	TYR	407	22.130	42.493	22.736	1.00	28.45
	ATOM	3105	CB	TYR	407	22.613	41.643	21.558	1.00	26.86
	ATOM	3106	CG	TYR	407	21.831	40.373	21.341	1.00	25.29
	ATOM	3107	CD1	TYR	407	20.700	40.358	20.535	1.00	25.44
45	ATOM	3108	CE1	TYR	407	19.964	39.189	20.346	1.00	25.93
	ATOM	3109	CD2	TYR	407	22.213	39.192	21.955	1.00	24.93
	ATOM	3110	CE2	TYR	407	21.488	38.021	21.780	1.00	25.18
	ATOM	3111	CZ	TYR	407	20.362	38.024	20.974	1.00	26.03
	ATOM	3112	OH	TYR	407	19.626	36.868	20.822	1.00	25.67
50	ATOM	3113	C	TYR	407	22.175	41.651	24.014	1.00	28.83
	ATOM	3114	O	TYR	407	21.202	40.988	24.369	1.00	28.62
	ATOM	3115	N	LYS	408	23.306	41.674	24.705	1.00	29.64
	ATOM	3116	CA	LYS	408	23.440	40.881	25.916	1.00	30.07
	ATOM	3117	CB	LYS	408	24.904	40.477	26.118	1.00	30.08
55	ATOM	3118	CG	LYS	408	25.442	39.556	25.030	1.00	30.61
	ATOM	3119	CD	LYS	408	26.597	38.698	25.529	1.00	30.05
	ATOM	3120	CE	LYS	408	26.799	37.515	24.601	1.00	30.22
	ATOM	3121	NZ	LYS	408	27.828	36.573	25.097	1.00	30.20
	ATOM	3122	C	LYS	408	22.940	41.551	27.185	1.00	30.82

Figure 4

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	ATOM	3123	O	LYS	408	22.327	40.901	28.038	1.00	31.98
	ATOM	3124	N	LEU	409	23.176	42.853	27.296	1.00	30.97
	ATOM	3125	CA	LEU	409	22.823	43.598	28.501	1.00	31.11
	ATOM	3126	CB	LEU	409	24.006	44.482	28.875	1.00	30.54
5	ATOM	3127	CG	LEU	409	25.305	43.700	28.962	1.00	29.31
	ATOM	3128	CD1	LEU	409	26.372	44.591	29.597	1.00	29.41
	ATOM	3129	CD2	LEU	409	25.067	42.423	29.785	1.00	28.16
	ATOM	3130	C	LEU	409	21.548	44.441	28.611	1.00	31.44
	ATOM	3131	O	LEU	409	20.978	44.542	29.708	1.00	31.86
10	ATOM	3132	N	HIS	410	21.122	45.077	27.519	1.00	31.34
	ATOM	3133	CA	HIS	410	19.929	45.912	27.572	1.00	30.80
	ATOM	3134	CB	HIS	410	19.732	46.635	26.247	1.00	30.36
	ATOM	3135	CG	HIS	410	18.703	47.717	26.303	1.00	29.89
	ATOM	3136	CD2	HIS	410	18.815	49.060	26.179	1.00	29.29
15	ATOM	3137	ND1	HIS	410	17.362	47.457	26.508	1.00	30.79
	ATOM	3138	CE1	HIS	410	16.691	48.595	26.505	1.00	29.88
	ATOM	3139	NE2	HIS	410	17.548	49.583	26.309	1.00	30.87
	ATOM	3140	C	HIS	410	18.728	45.031	27.900	1.00	31.41
	ATOM	3141	O	HIS	410	18.467	44.055	27.207	1.00	31.97
20	ATOM	3142	N	PRO	411	17.985	45.376	28.969	1.00	31.63
	ATOM	3143	CD	PRO	411	18.173	46.690	29.610	1.00	31.32
	ATOM	3144	CA	PRO	411	16.798	44.708	29.518	1.00	31.33
	ATOM	3145	CB	PRO	411	16.111	45.815	30.299	1.00	31.27
	ATOM	3146	CG	PRO	411	17.257	46.599	30.822	1.00	32.32
25	ATOM	3147	C	PRO	411	15.827	44.037	28.571	1.00	32.09
	ATOM	3148	O	PRO	411	15.362	42.920	28.838	1.00	32.76
	ATOM	3149	N	SER	412	15.519	44.684	27.457	1.00	31.73
	ATOM	3150	CA	SER	412	14.527	44.094	26.573	1.00	31.92
	ATOM	3151	CB	SER	412	13.210	44.834	26.771	1.00	32.51
30	ATOM	3152	OG	SER	412	13.368	46.200	26.390	1.00	33.27
	ATOM	3153	C	SER	412	14.838	44.047	25.082	1.00	31.91
	ATOM	3154	O	SER	412	14.039	43.520	24.304	1.00	32.59
	ATOM	3155	N	PHE	413	15.974	44.601	24.679	1.00	30.72
	ATOM	3156	CA	PHE	413	16.348	44.615	23.271	1.00	30.13
35	ATOM	3157	CB	PHE	413	17.778	45.105	23.130	1.00	28.18
	ATOM	3158	CG	PHE	413	18.213	45.285	21.716	1.00	25.96
	ATOM	3159	CD1	PHE	413	18.085	46.522	21.094	1.00	25.70
	ATOM	3160	CD2	PHE	413	18.772	44.233	21.015	1.00	24.47
	ATOM	3161	CE1	PHE	413	18.517	46.711	19.787	1.00	25.13
40	ATOM	3162	CE2	PHE	413	19.208	44.408	19.707	1.00	24.84
	ATOM	3163	CZ	PHE	413	19.082	45.652	19.092	1.00	24.48
	ATOM	3164	C	PHE	413	16.232	43.228	22.645	1.00	31.20
	ATOM	3165	O	PHE	413	15.571	43.026	21.612	1.00	31.56
	ATOM	3166	N	LYS	414	16.888	42.268	23.275	1.00	31.75
45	ATOM	3167	CA	LYS	414	16.851	40.906	22.790	1.00	32.75
	ATOM	3168	CB	LYS	414	17.626	39.999	23.755	1.00	33.66
	ATOM	3169	CG	LYS	414	17.570	38.526	23.429	1.00	34.45
	ATOM	3170	CD	LYS	414	18.732	37.744	24.049	1.00	36.05
	ATOM	3171	CE	LYS	414	18.845	37.909	25.558	1.00	35.80
50	ATOM	3172	NZ	LYS	414	19.972	38.817	25.920	1.00	36.66
	ATOM	3173	C	LYS	414	15.412	40.411	22.600	1.00	33.19
	ATOM	3174	O	LYS	414	15.054	39.927	21.518	1.00	33.30
	ATOM	3175	N	GLU	415	14.577	40.542	23.627	1.00	33.81
	ATOM	3176	CA	GLU	415	13.193	40.071	23.513	1.00	34.53
55	ATOM	3177	CB	GLU	415	12.462	40.251	24.838	1.00	37.66
	ATOM	3178	CG	GLU	415	13.062	39.497	26.002	1.00	42.83
	ATOM	3179	CD	GLU	415	14.376	40.090	26.520	1.00	45.68
	ATOM	3180	OE1	GLU	415	14.523	41.339	26.526	1.00	47.31
	ATOM	3181	OE2	GLU	415	15.245	39.293	26.956	1.00	47.44

Figure 4

	ATOM	3182	C	GLU	415	12.409	40.776	22.401	1.00	33.23
	ATOM	3183	O	GLU	415	11.676	40.137	21.649	1.00	33.06
	ATOM	3184	N	ARG	416	12.551	42.092	22.299	1.00	31.77
	ATOM	3185	CA	ARG	416	11.841	42.825	21.264	1.00	30.32
5	ATOM	3186	CB	ARG	416	12.066	44.328	21.427	1.00	31.27
	ATOM	3187	CG	ARG	416	11.645	44.875	22.796	1.00	33.92
	ATOM	3188	CD	ARG	416	11.783	46.393	22.901	1.00	35.48
	ATOM	3189	NE	ARG	416	11.545	46.866	24.267	1.00	38.24
	ATOM	3190	CZ	ARG	416	11.982	48.030	24.746	1.00	39.11
10	ATOM	3191	NH1	ARG	416	12.676	48.850	23.967	1.00	39.89
	ATOM	3192	NH2	ARG	416	11.754	48.365	26.009	1.00	38.52
	ATOM	3193	C	ARG	416	12.379	42.354	19.916	1.00	29.08
	ATOM	3194	O	ARG	416	11.620	42.159	18.964	1.00	28.85
	ATOM	3195	N	PHE	417	13.694	42.144	19.862	1.00	27.59
15	ATOM	3196	CA	PHE	417	14.377	41.707	18.648	1.00	25.70
	ATOM	3197	CB	PHE	417	15.886	41.687	18.890	1.00	23.64
	ATOM	3198	CG	PHE	417	16.687	41.310	17.680	1.00	20.59
	ATOM	3199	CD1	PHE	417	16.910	42.230	16.671	1.00	18.99
	ATOM	3200	CD2	PHE	417	17.183	40.018	17.540	1.00	19.41
20	ATOM	3201	CE1	PHE	417	17.610	41.870	15.540	1.00	19.87
	ATOM	3202	CE2	PHE	417	17.884	39.641	16.413	1.00	18.04
	ATOM	3203	CZ	PHE	417	18.100	40.563	15.409	1.00	20.04
	ATOM	3204	C	PHE	417	13.943	40.342	18.099	1.00	25.74
	ATOM	3205	O	PHE	417	13.568	40.225	16.927	1.00	25.24
25	ATOM	3206	N	HIS	418	14.012	39.301	18.922	1.00	26.11
	ATOM	3207	CA	HIS	418	13.612	37.962	18.459	1.00	26.79
	ATOM	3208	CB	HIS	418	13.638	36.973	19.615	1.00	28.01
	ATOM	3209	CG	HIS	418	14.973	36.854	20.279	1.00	28.81
	ATOM	3210	CD2	HIS	418	16.168	37.425	19.989	1.00	29.42
30	ATOM	3211	ND1	HIS	418	15.182	36.067	21.389	1.00	28.15
	ATOM	3212	CE1	HIS	418	16.446	36.157	21.755	1.00	29.43
	ATOM	3213	NE2	HIS	418	17.067	36.974	20.924	1.00	29.74
	ATOM	3214	C	HIS	418	12.209	37.985	17.876	1.00	26.41
	ATOM	3215	O	HIS	418	11.976	37.565	16.733	1.00	26.40
35	ATOM	3216	N	ALA	419	11.284	38.487	18.688	1.00	25.83
	ATOM	3217	CA	ALA	419	9.885	38.603	18.328	1.00	25.05
	ATOM	3218	CB	ALA	419	9.182	39.454	19.352	1.00	24.80
	ATOM	3219	C	ALA	419	9.731	39.215	16.943	1.00	25.35
	ATOM	3220	O	ALA	419	9.146	38.601	16.029	1.00	25.99
40	ATOM	3221	N	SER	420	10.249	40.425	16.777	1.00	25.26
	ATOM	3222	CA	SER	420	10.159	41.078	15.481	1.00	25.31
	ATOM	3223	CB	SER	420	10.897	42.405	15.515	1.00	23.85
	ATOM	3224	OG	SER	420	10.692	43.089	14.303	1.00	23.43
	ATOM	3225	C	SER	420	10.751	40.170	14.391	1.00	26.14
45	ATOM	3226	O	SER	420	10.145	39.976	13.331	1.00	25.95
	ATOM	3227	N	VAL	421	11.926	39.602	14.670	1.00	27.34
	ATOM	3228	CA	VAL	421	12.602	38.699	13.733	1.00	28.41
	ATOM	3229	CB	VAL	421	13.919	38.127	14.346	1.00	27.63
	ATOM	3230	CG1	VAL	421	14.479	37.020	13.475	1.00	26.36
50	ATOM	3231	CG2	VAL	421	14.953	39.232	14.469	1.00	28.22
	ATOM	3232	C	VAL	421	11.689	37.535	13.325	1.00	29.65
	ATOM	3233	O	VAL	421	11.557	37.227	12.130	1.00	28.72
	ATOM	3234	N	ARG	422	11.069	36.886	14.310	1.00	30.74
	ATOM	3235	CA	ARG	422	10.165	35.775	14.014	1.00	32.79
55	ATOM	3236	CB	ARG	422	9.419	35.328	15.265	1.00	33.29
	ATOM	3237	CG	ARG	422	10.259	35.197	16.512	1.00	34.47
	ATOM	3238	CD	ARG	422	11.081	33.927	16.558	1.00	34.54
	ATOM	3239	NE	ARG	422	11.862	33.905	17.795	1.00	35.75
	ATOM	3240	CZ	ARG	422	12.824	33.028	18.066	1.00	35.45

Figure 4

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	ATOM	3241	NH1	ARG	422	13.127	32.085	17.180	1.00	35.35
	ATOM	3242	NH2	ARG	422	13.490	33.108	19.215	1.00	33.55
	ATOM	3243	C	ARG	422	9.123	36.277	13.019	1.00	33.41
	ATOM	3244	O	ARG	422	8.949	35.728	11.929	1.00	33.68
5	ATOM	3245	N	ARG	423	8.446	37.348	13.417	1.00	34.00
	ATOM	3246	CA	ARG	423	7.394	37.946	12.622	1.00	34.13
	ATOM	3247	CB	ARG	423	7.022	39.301	13.207	1.00	35.16
	ATOM	3248	CG	ARG	423	5.538	39.584	13.202	1.00	36.10
	ATOM	3249	CD	ARG	423	5.212	40.831	14.012	1.00	37.57
10	ATOM	3250	NE	ARG	423	5.482	40.682	15.441	1.00	38.90
	ATOM	3251	CZ	ARG	423	6.274	41.503	16.133	1.00	40.51
	ATOM	3252	NH1	ARG	423	6.874	42.523	15.513	1.00	41.42
	ATOM	3253	NH2	ARG	423	6.461	41.324	17.440	1.00	38.76
	ATOM	3254	C	ARG	423	7.754	38.100	11.165	1.00	33.94
15	ATOM	3255	O	ARG	423	6.919	37.849	10.295	1.00	35.59
	ATOM	3256	N	LEU	424	8.993	38.494	10.884	1.00	32.85
	ATOM	3257	CA	LEU	424	9.418	38.699	9.497	1.00	31.57
	ATOM	3258	CB	LEU	424	10.474	39.788	9.450	1.00	28.75
	ATOM	3259	CG	LEU	424	10.030	41.129	10.003	1.00	27.64
20	ATOM	3260	CD1	LEU	424	11.220	42.080	10.066	1.00	26.47
	ATOM	3261	CD2	LEU	424	8.942	41.686	9.115	1.00	27.23
	ATOM	3262	C	LEU	424	9.950	37.479	8.747	1.00	32.00
	ATOM	3263	O	LEU	424	10.232	37.562	7.551	1.00	31.15
	ATOM	3264	N	THR	425	10.065	36.343	9.424	1.00	33.88
25	ATOM	3265	CA	THR	425	10.615	35.153	8.778	1.00	35.30
	ATOM	3266	CB	THR	425	11.886	34.722	9.495	1.00	35.17
	ATOM	3267	OG1	THR	425	11.580	34.463	10.874	1.00	35.24
	ATOM	3268	CG2	THR	425	12.939	35.817	9.399	1.00	35.16
	ATOM	3269	C	THR	425	9.711	33.923	8.675	1.00	37.00
30	ATOM	3270	O	THR	425	10.059	32.854	9.182	1.00	37.54
	ATOM	3271	N	PRO	426	8.562	34.040	7.982	1.00	38.04
	ATOM	3272	CD	PRO	426	8.144	35.123	7.073	1.00	38.49
	ATOM	3273	CA	PRO	426	7.663	32.890	7.856	1.00	38.85
	ATOM	3274	CB	PRO	426	6.745	33.295	6.700	1.00	38.23
35	ATOM	3275	CG	PRO	426	6.699	34.772	6.802	1.00	38.07
	ATOM	3276	C	PRO	426	8.445	31.615	7.527	1.00	39.83
	ATOM	3277	O	PRO	426	9.378	31.641	6.728	1.00	40.28
	ATOM	3278	N	SER	427	8.073	30.510	8.158	1.00	40.72
	ATOM	3279	CA	SER	427	8.713	29.232	7.892	1.00	41.82
40	ATOM	3280	CB	SER	427	8.358	28.785	6.474	1.00	42.86
	ATOM	3281	OG	SER	427	6.954	28.802	6.287	1.00	44.69
	ATOM	3282	C	SER	427	10.234	29.228	8.068	1.00	42.10
	ATOM	3283	O	SER	427	10.981	28.899	7.140	1.00	41.85
	ATOM	3284	N	CYS	428	10.679	29.586	9.267	1.00	42.60
45	ATOM	3285	CA	CYS	428	12.096	29.608	9.601	1.00	42.43
	ATOM	3286	CB	CYS	428	12.724	30.960	9.258	1.00	42.59
	ATOM	3287	SG	CYS	428	12.860	31.327	7.492	1.00	44.02
	ATOM	3288	C	CYS	428	12.195	29.381	11.096	1.00	42.45
	ATOM	3289	O	CYS	428	11.671	30.169	11.879	1.00	43.76
50	ATOM	3290	N	GLU	429	12.846	28.296	11.494	1.00	42.34
	ATOM	3291	CA	GLU	429	13.014	27.995	12.909	1.00	41.23
	ATOM	3292	CB	GLU	429	13.030	26.486	13.146	1.00	42.97
	ATOM	3293	CG	GLU	429	11.699	25.796	12.933	1.00	45.48
	ATOM	3294	CD	GLU	429	11.847	24.282	12.925	1.00	47.43
55	ATOM	3295	OE1	GLU	429	12.518	23.756	13.847	1.00	48.77
	ATOM	3296	OE2	GLU	429	11.298	23.623	12.005	1.00	48.07
	ATOM	3297	C	GLU	429	14.341	28.587	13.346	1.00	39.77
	ATOM	3298	O	GLU	429	15.370	27.902	13.352	1.00	39.92
	ATOM	3299	N	ILE	430	14.315	29.864	13.708	1.00	38.09

Figure 4

ATOM	3300	CA	ILE	430	15.514	30.560	14.142	1.00	36.48
ATOM	3301	CB	ILE	430	15.341	32.070	13.998	1.00	35.17
ATOM	3302	CG2	ILE	430	16.659	32.770	14.280	1.00	34.48
ATOM	3303	CG1	ILE	430	14.839	32.390	12.589	1.00	35.30
ATOM	3304	CD1	ILE	430	14.669	33.866	12.310	1.00	34.88
ATOM	3305	C	ILE	430	15.872	30.254	15.591	1.00	37.06
ATOM	3306	O	ILE	430	15.044	30.399	16.495	1.00	38.13
ATOM	3307	N	THR	431	17.109	29.823	15.808	1.00	36.61
ATOM	3308	CA	THR	431	17.600	29.520	17.146	1.00	36.17
ATOM	3309	CB	THR	431	18.067	28.053	17.240	1.00	36.58
ATOM	3310	OG1	THR	431	16.950	27.180	17.031	1.00	36.34
ATOM	3311	CG2	THR	431	18.692	27.774	18.604	1.00	36.38
ATOM	3312	C	THR	431	18.796	30.441	17.396	1.00	36.13
ATOM	3313	O	THR	431	19.705	30.513	16.569	1.00	36.10
ATOM	3314	N	PHE	432	18.804	31.157	18.514	1.00	35.79
ATOM	3315	CA	PHE	432	19.926	32.054	18.794	1.00	35.93
ATOM	3316	CB	PHE	432	19.443	33.450	19.232	1.00	34.31
ATOM	3317	CG	PHE	432	18.643	34.194	18.188	1.00	32.53
ATOM	3318	CD1	PHE	432	17.271	33.977	18.048	1.00	31.59
ATOM	3319	CD2	PHE	432	19.262	35.124	17.353	1.00	31.00
ATOM	3320	CE1	PHE	432	16.527	34.676	17.092	1.00	30.53
ATOM	3321	CE2	PHE	432	18.525	35.826	16.395	1.00	30.25
ATOM	3322	CZ	PHE	432	17.154	35.600	16.266	1.00	30.11
ATOM	3323	C	PHE	432	20.767	31.483	19.917	1.00	37.08
ATOM	3324	O	PHE	432	20.248	30.772	20.779	1.00	38.85
ATOM	3325	N	ILE	433	22.063	31.774	19.906	1.00	37.32
ATOM	3326	CA	ILE	433	22.933	31.321	20.983	1.00	38.46
ATOM	3327	CB	ILE	433	23.526	29.890	20.722	1.00	39.06
ATOM	3328	CG2	ILE	433	22.398	28.863	20.624	1.00	38.62
ATOM	3329	CG1	ILE	433	24.367	29.861	19.449	1.00	39.03
ATOM	3330	CD1	ILE	433	25.028	28.520	19.227	1.00	38.32
ATOM	3331	C	ILE	433	24.039	32.358	21.161	1.00	39.33
ATOM	3332	O	ILE	433	24.429	33.034	20.201	1.00	39.15
ATOM	3333	N	GLU	434	24.527	32.505	22.388	1.00	40.58
ATOM	3334	CA	GLU	434	25.559	33.498	22.669	1.00	42.92
ATOM	3335	CB	GLU	434	25.152	34.312	23.885	1.00	43.91
ATOM	3336	CG	GLU	434	23.769	34.883	23.744	1.00	45.53
ATOM	3337	CD	GLU	434	23.342	35.640	24.965	1.00	46.68
ATOM	3338	OE1	GLU	434	23.436	35.072	26.074	1.00	47.18
ATOM	3339	OE2	GLU	434	22.910	36.802	24.816	1.00	48.77
ATOM	3340	C	GLU	434	26.965	32.950	22.865	1.00	44.01
ATOM	3341	O	GLU	434	27.206	32.058	23.680	1.00	44.48
ATOM	3342	N	SER	435	27.901	33.518	22.119	1.00	45.00
ATOM	3343	CA	SER	435	29.284	33.075	22.167	1.00	46.11
ATOM	3344	CB	SER	435	30.077	33.779	21.057	1.00	46.95
ATOM	3345	OG	SER	435	29.839	35.186	21.053	1.00	47.94
ATOM	3346	C	SER	435	29.984	33.274	23.507	1.00	46.36
ATOM	3347	O	SER	435	30.043	34.396	24.022	1.00	46.31
ATOM	3348	N	GLU	436	30.505	32.180	24.069	1.00	46.22
ATOM	3349	CA	GLU	436	31.248	32.250	25.330	1.00	46.33
ATOM	3350	CB	GLU	436	31.322	30.884	26.020	1.00	47.64
ATOM	3351	CG	GLU	436	32.144	30.908	27.317	1.00	50.83
ATOM	3352	CD	GLU	436	32.726	29.541	27.711	1.00	52.03
ATOM	3353	OE1	GLU	436	31.951	28.585	27.970	1.00	52.84
ATOM	3354	OE2	GLU	436	33.972	29.428	27.765	1.00	52.07
ATOM	3355	C	GLU	436	32.650	32.671	24.912	1.00	45.58
ATOM	3356	O	GLU	436	33.446	31.843	24.463	1.00	45.50
ATOM	3357	N	GLU	437	32.950	33.956	25.051	1.00	44.67
ATOM	3358	CA	GLU	437	34.252	34.462	24.643	1.00	44.13

Figure 4

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	ATOM	3359	CB	GLU	437	35.328	34.050	25.652	1.00	43.61
	ATOM	3360	CG	GLU	437	36.745	34.334	25.190	1.00	43.39
	ATOM	3361	CD	GLU	437	36.931	35.752	24.678	1.00	43.50
	ATOM	3362	OE1	GLU	437	36.976	36.680	25.514	1.00	44.49
5	ATOM	3363	OE2	GLU	437	37.025	35.940	23.441	1.00	42.17
	ATOM	3364	C	GLU	437	34.569	33.880	23.264	1.00	43.56
	ATOM	3365	O	GLU	437	35.530	33.131	23.108	1.00	45.30
	ATOM	3366	N	GLY	438	33.757	34.225	22.266	1.00	41.68
	ATOM	3367	CA	GLY	438	33.958	33.700	20.926	1.00	39.44
10	ATOM	3368	C	GLY	438	34.748	34.538	19.934	1.00	38.11
	ATOM	3369	O	GLY	438	34.932	34.130	18.791	1.00	37.45
	ATOM	3370	N	SER	439	35.213	35.713	20.329	1.00	37.14
	ATOM	3371	CA	SER	439	35.980	36.502	19.386	1.00	36.86
	ATOM	3372	CB	SER	439	35.916	37.983	19.714	1.00	36.81
15	ATOM	3373	OG	SER	439	36.825	38.678	18.878	1.00	35.32
	ATOM	3374	C	SER	439	37.420	36.053	19.444	1.00	36.74
	ATOM	3375	O	SER	439	38.192	36.265	18.513	1.00	36.37
	ATOM	3376	N	GLY	440	37.774	35.439	20.562	1.00	36.58
	ATOM	3377	CA	GLY	440	39.126	34.957	20.746	1.00	36.42
20	ATOM	3378	C	GLY	440	39.207	33.518	20.302	1.00	36.28
	ATOM	3379	O	GLY	440	40.146	33.140	19.613	1.00	36.20
	ATOM	3380	N	ARG	441	38.224	32.714	20.699	1.00	36.09
	ATOM	3381	CA	ARG	441	38.190	31.309	20.312	1.00	37.16
	ATOM	3382	CB	ARG	441	37.151	30.562	21.138	1.00	37.34
25	ATOM	3383	CG	ARG	441	37.312	30.717	22.632	1.00	39.57
	ATOM	3384	CD	ARG	441	36.334	29.806	23.375	1.00	42.28
	ATOM	3385	NE	ARG	441	35.270	29.339	22.488	1.00	44.36
	ATOM	3386	CZ	ARG	441	34.240	28.585	22.862	1.00	45.80
	ATOM	3387	NH1	ARG	441	34.103	28.192	24.127	1.00	45.87
30	ATOM	3388	NH2	ARG	441	33.346	28.214	21.955	1.00	47.26
	ATOM	3389	C	ARG	441	37.848	31.179	18.821	1.00	37.42
	ATOM	3390	O	ARG	441	38.103	30.151	18.189	1.00	37.52
	ATOM	3391	N	GLY	442	37.270	32.234	18.262	1.00	37.34
	ATOM	3392	CA	GLY	442	36.906	32.204	16.863	1.00	37.39
35	ATOM	3393	C	GLY	442	38.165	32.308	16.048	1.00	37.47
	ATOM	3394	O	GLY	442	38.483	31.410	15.278	1.00	37.51
	ATOM	3395	N	ALA	443	38.887	33.408	16.241	1.00	38.17
	ATOM	3396	CA	ALA	443	40.134	33.660	15.526	1.00	38.50
	ATOM	3397	CB	ALA	443	40.739	34.999	15.967	1.00	36.50
40	ATOM	3398	C	ALA	443	41.127	32.521	15.759	1.00	39.03
	ATOM	3399	O	ALA	443	42.015	32.297	14.941	1.00	39.36
	ATOM	3400	N	ALA	444	40.977	31.807	16.875	1.00	39.93
	ATOM	3401	CA	ALA	444	41.864	30.685	17.172	1.00	40.31
	ATOM	3402	CB	ALA	444	41.724	30.242	18.623	1.00	39.25
45	ATOM	3403	C	ALA	444	41.427	29.569	16.246	1.00	40.97
	ATOM	3404	O	ALA	444	42.146	29.210	15.312	1.00	41.31
	ATOM	3405	N	LEU	445	40.233	29.038	16.501	1.00	41.41
	ATOM	3406	CA	LEU	445	39.678	27.960	15.690	1.00	41.97
	ATOM	3407	CB	LEU	445	38.195	27.776	16.024	1.00	40.09
50	ATOM	3408	CG	LEU	445	37.954	26.806	17.182	1.00	39.14
	ATOM	3409	CD1	LEU	445	36.750	27.233	17.982	1.00	39.27
	ATOM	3410	CD2	LEU	445	37.781	25.399	16.647	1.00	37.36
	ATOM	3411	C	LEU	445	39.860	28.156	14.176	1.00	43.29
	ATOM	3412	O	LEU	445	39.918	27.179	13.427	1.00	43.28
55	ATOM	3413	N	VAL	446	39.955	29.406	13.729	1.00	44.66
	ATOM	3414	CA	VAL	446	40.136	29.684	12.307	1.00	46.32
	ATOM	3415	CB	VAL	446	39.687	31.120	11.948	1.00	46.15
	ATOM	3416	CG1	VAL	446	40.356	31.578	10.653	1.00	46.15
	ATOM	3417	CG2	VAL	446	38.164	31.160	11.793	1.00	45.75

Figure 4

	ATOM	3418	C	VAL	446	41.597	29.503	11.944	1.00	48.03
	ATOM	3419	O	VAL	446	41.929	29.105	10.825	1.00	48.75
	ATOM	3420	N	SER	447	42.465	29.802	12.904	1.00	49.63
	ATOM	3421	CA	SER	447	43.902	29.657	12.725	1.00	50.76
5	ATOM	3422	CB	SER	447	44.635	30.267	13.918	1.00	50.76
	ATOM	3423	OG	SER	447	44.377	31.659	14.021	1.00	50.83
	ATOM	3424	C	SER	447	44.259	28.173	12.612	1.00	52.07
	ATOM	3425	O	SER	447	44.923	27.753	11.662	1.00	52.17
	ATOM	3426	N	ALA	448	43.804	27.387	13.584	1.00	53.51
10	ATOM	3427	CA	ALA	448	44.071	25.953	13.621	1.00	55.46
	ATOM	3428	CB	ALA	448	43.273	25.306	14.745	1.00	55.02
	ATOM	3429	C	ALA	448	43.751	25.263	12.300	1.00	57.02
	ATOM	3430	O	ALA	448	44.599	24.564	11.726	1.00	57.18
	ATOM	3431	N	VAL	449	42.523	25.457	11.825	1.00	58.39
15	ATOM	3432	CA	VAL	449	42.093	24.841	10.579	1.00	59.69
	ATOM	3433	CB	VAL	449	40.571	24.977	10.382	1.00	59.67
	ATOM	3434	CG1	VAL	449	40.152	24.262	9.112	1.00	60.28
	ATOM	3435	CG2	VAL	449	39.833	24.384	11.577	1.00	59.48
	ATOM	3436	C	VAL	449	42.821	25.482	9.403	1.00	60.70
20	ATOM	3437	O	VAL	449	42.903	24.898	8.321	1.00	61.00
	ATOM	3438	N	ALA	450	43.361	26.677	9.627	1.00	61.41
	ATOM	3439	CA	ALA	450	44.093	27.392	8.591	1.00	62.12
	ATOM	3440	CB	ALA	450	43.981	28.889	8.814	1.00	62.32
	ATOM	3441	C	ALA	450	45.558	26.973	8.606	1.00	63.02
25	ATOM	3442	O	ALA	450	46.437	27.748	8.217	1.00	62.75
	ATOM	3443	N	CYS	451	45.807	25.744	9.061	1.00	64.03
	ATOM	3444	CA	CYS	451	47.160	25.183	9.148	1.00	65.19
	ATOM	3445	CB	CYS	451	47.530	24.440	7.850	1.00	65.75
	ATOM	3446	SG	CYS	451	46.901	22.720	7.723	1.00	66.86
30	ATOM	3447	C	CYS	451	48.239	26.217	9.474	1.00	65.22
	ATOM	3448	O	CYS	451	47.929	27.230	10.144	1.00	65.18
	ATOM	3449	OXT	CYS	451	49.398	25.979	9.073	1.00	65.50
	ATOM	3450	C1	HEX	1	31.023	47.521	12.611	1.00	25.83
	ATOM	3451	C2	HEX	1	32.239	47.182	11.801	1.00	25.25
35	ATOM	3452	C3	HEX	1	32.203	45.697	11.565	1.00	25.11
	ATOM	3453	C4	HEX	1	32.071	44.939	12.862	1.00	24.99
	ATOM	3454	C5	HEX	1	31.030	45.591	13.785	1.00	25.34
	ATOM	3455	C6	HEX	1	30.772	44.921	15.126	1.00	25.58
	ATOM	3456	O1	HEX	1	30.750	48.942	12.579	1.00	27.04
40	ATOM	3457	O2	HEX	1	32.183	47.912	10.609	1.00	24.71
	ATOM	3458	O3	HEX	1	33.337	45.251	10.836	1.00	25.99
	ATOM	3459	O4	HEX	1	31.699	43.621	12.545	1.00	25.85
	ATOM	3460	O5	HEX	1	31.267	46.968	13.935	1.00	25.37
	ATOM	3461	O6	HEX	1	31.835	45.222	16.009	1.00	27.23
45	ATOM	3462	C1	LIG	1	30.034	26.620	8.669	1.00	35.87
	ATOM	3463	C2	LIG	1	29.909	27.259	10.064	1.00	34.82
	ATOM	3464	C3	LIG	1	31.308	27.852	10.344	1.00	35.54
	ATOM	3465	C4	LIG	1	32.212	27.447	9.148	1.00	35.52
	ATOM	3466	C5	LIG	1	31.520	26.207	8.584	1.00	35.20
50	ATOM	3467	C6	LIG	1	33.670	27.245	9.637	1.00	36.33
	ATOM	3468	C7	LIG	1	34.562	26.321	8.758	1.00	37.11
	ATOM	3469	C8	LIG	1	35.946	26.832	8.778	1.00	36.91
	ATOM	3470	N9	LIG	1	36.382	27.317	7.570	1.00	36.92
	ATOM	3471	C10	LIG	1	37.668	27.907	7.331	1.00	36.42
55	ATOM	3472	N11	LIG	1	38.035	28.336	6.087	1.00	37.39
	ATOM	3473	C12	LIG	1	39.058	28.930	6.462	1.00	36.99
	ATOM	3474	C13	LIG	1	39.426	29.003	7.575	1.00	37.10
	ATOM	3475	S14	LIG	1	38.681	28.342	8.700	1.00	37.86
	ATOM	3476	O15	LIG	1	36.640	26.843	9.817	1.00	38.32

Figure 4

```
ATOM    3477   C16 LIG      1     34.538  24.890   9.296  1.00 37.59
ATOM    3478   C17 LIG      1     34.906  24.620  10.610  1.00 37.22
ATOM    3479   C18 LIG      1     34.658  23.346  11.130  1.00 38.09
ATOM    3480   N19 LIG      1     34.084  22.371  10.404  1.00 38.80
ATOM    3481   C20 LIG      1     33.729  22.598   9.128  1.00 38.90
ATOM    3482   C21 LIG      1     33.942  23.860   8.546  1.00 38.73
ATOM    3483   K1  K        1     32.471  32.037  -7.104  1.00 46.91
END
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CRYSTALS OF GLUCOKINASE AND METHODS OF GROWING THEM

The invention relates to crystalline forms of Glucokinase of sufficient size and quality to obtain structural data by X-ray crystallography and to methods of growing such crystals.

5

Glucokinase (GK) is one of four hexokinases found in mammals [Colowick, S.P., in *The Enzymes*, Vol. 9 (P. Boyer, ed.) Academic Press, New York, NY, pages 1-48, 1973]. The hexokinases catalyze the first step in the metabolism of glucose, i.e., the conversion of glucose to glucose-6-phosphate. Glucokinase has a limited cellular

10 distribution, being found principally in pancreatic β-cells and liver parenchymal cells. In addition, GK is a rate-controlling enzyme for glucose metabolism in these two cell types that are known to play critical roles in whole-body glucose homeostasis [Chipkin, S.R., Kelly, K.L., and Ruderman, N.B. in *Joslin's Diabetes* (C.R. Khan and G.C. Wier, eds.), Lea and Febiger, Philadelphia, PA, pages 97-115, 1994]. The concentration of glucose at

15 which GK demonstrates half-maximal activity is approximately 8 mM. The other three hexokinases are saturated with glucose at much lower concentrations (<1 mM). Therefore, the flux of glucose through the GK pathway rises as the concentration of glucose in the blood increases from fasting (5 mM) to postprandial (≈10-15 mM) levels following a carbohydrate-containing meal [Printz, R.G., Magnuson, M.A., and Granner,

20 D.K. in *Ann. Rev. Nutrition* Vol. 13 (R.E. Olson, D.M. Bier, and D.B. McCormick, eds.), Annual Review, Inc., Palo Alto, CA, pages 463-496, 1993]. These findings contributed over a decade ago to the hypothesis that GK functions as a glucose sensor in β-cells and hepatocytes (Meglasson, M.D. and Matschinsky, F.M. *Amer. J. Physiol.* 246, E1-E13, 1984). In recent years, studies in transgenic animals have confirmed that GK does indeed

25 play a critical role in whole-body glucose homeostasis. Animals that do not express GK die within days of birth with severe diabetes while animals overexpressing GK have improved glucose tolerance (Grupe, A., Hultgren, B., Ryan, A. et al., *Cell* 83, 69-78, 1995; Ferrie, T., Riu, E., Bosch, F. et al., *FASEB J.*, 10, 1213-1218, 1996). An increase in glucose exposure is coupled through GK in β-cells to increased insulin secretion and in

30 hepatocytes to increased glycogen deposition and perhaps decreased glucose production.

The finding that type II maturity-onset diabetes of the young (MODY-2) is caused by loss of function mutations in the GK gene suggests that GK also functions as a glucose sensor in humans (Liang, Y., Kesavan, P., Wang, L. et al., *Biochem. J.* 309, 167-173, 1995). Additional evidence supporting an important role for GK in the regulation of glucose metabolism in humans was provided by the identification of patients that express a mutant form of GK with increased enzymatic activity. These patients exhibit a fasting hypoglycemia associated with an inappropriately elevated level of plasma insulin (Glaser, B., Kesavan, P., Heyman, M. et al., *New England J. Med.* 338, 226-230, 1998). While mutations of the GK gene are not found in the majority of patients with type II diabetes, compounds that activate GK and, thereby, increase the sensitivity of the GK sensor system will still be useful in the treatment of the hyperglycemia characteristic of all type II diabetes. Glucokinase activators will increase the flux of glucose metabolism in β-cells and hepatocytes, which will be coupled to increased insulin secretion. Such agents would be useful for treating type II diabetes.

In an effort to elucidate the mechanisms underlying kinase activation , the crystal structure of such proteins is often sought to be determined. The crystal structures of several hexokinases have been reported. See, e.g. A. E. Aleshin, C. Zeng, G. P. Bourenkov, H. D. Bartunik, H. J. Fromm & R. B. Honzatko 'The mechanism of regulation of hexokinase: new insights from the crystal structure of recombinant human brain hexokinase complexed with glucose and glucose-6-phosphate' *Structure* 6, 39-50 (1998); W. S. Bennett, Jr. & T. A. Steitz 'Structure of a complex between yeast hexokinase A and glucose I. Structure determination and refinement at 3.5 Å resolution' *J. Mol. Biol.* 140, 183-209 (1978); and S. Ito, S. Fushinobu, I. Yoshioka, S. Koga, H. Matsuzawa & T. Wakagi 'Structural Basis for the ADP-Specificity of a Novel Glucokinase from a Hyperthermophilic Archaeon' *Structure* 9, 205-214 (2001). Despite these reports, researchers armed with the knowledge of how to obtain crystals of related hexokinases have attempted to obtain crystals of any mammalian Glucokinase without success.

Applicants have discovered protocols which allow crystallization of mammalian Glucokinase with or without a bound allosteric ligand. The crystal structure has been solved by X-ray crystallography to a resolution of 2.7 Å. See Figures 3 and 4. Thus the invention relates to a crystalline form of Glucokinase and a crystalline form of a complex

5   of Glucokinase and an allosteric ligand. The invention further relates to a method of forming crystals of Glucokinase, with or without a bound allosteric ligand.

Figure 1 shows Glucokinase co-crystals having P6(5)22 symmetry.

10   Figure 2 shows the amino acid sequence of an expressed Glucokinase used for crystallization.

Figure 3 shows a ribbon diagram of the structure of Glucokinase showing the α-helices and β-sheets.

15

Figure 4 shows the atomic structure coordinates for Glucokinase bound to 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide.

The present invention relates to crystalline forms of mammalian Glucokinase, with

20   or without a ligand bound in the allosteric site, where the crystals are of sufficient quality and size to allow for the determination of the three-dimensional X-ray diffraction structure to a resolution of about 2.0 Å to about 3.5 Å. The invention also relates to methods for preparing and crystallizing the Glucokinase. The crystalline forms of Glucokinase, as well as information derived from their crystal structures can be used to

25   analyze and modify glucokinase activity as well as to identify compounds that interact with the allosteric site.

- 3 -

The crystals of the invention include apo crystals and co-crystals. The apo crystals of the invention generally comprise substantially pure Glucokinase. The co-crystals generally comprise substantially pure Glucokinase with a ligand bound to the allosteric site.

5

It is to be understood that the crystalline Glucokinases of the invention are not limited to naturally occurring or native Glucokinases. Indeed, the crystals of the invention include mutants of the native Glucokinases. Mutants of native Glucokinases are obtained by replacing at least one amino acid residue in a native Glucokinase domain

10 with a different amino acid residue, or by adding or deleting amino acid residues within the native polypeptide or at the N- or C- terminus of the native polypeptide, and have substantially the same three-dimensional structure as the native Glucokinase from which the mutant is derived.

15 By having substantially the same three-dimensional structure is meant having a set of atomic structure coordinates from an apo- or co-crystal that have a root mean square deviation of less than or equal to about 2 Å when superimposed with the atomic structure coordinates of the native Glucokinase from which the mutant is derived when at least about 50% to about 100% of the alpha carbon atoms of the native Glucokinase are

20 included in the superposition.

In some instances, it may be particularly advantageous or convenient to substitute, delete and/or add amino acid residues to a native Glucokinase domain in order to provide convenient cloning sites in cDNA encoding the polypeptide, to aid in purification of the

25 polypeptide, etc. Such substitutions, deletions and/or additions which do not substantially alter the three dimensional structure of the native Glucokinase will be apparent to those having skills in the art.

It should be noted that the mutants contemplated herein need not exhibit glucokinase activity. Indeed, amino acid substitutions, additions or deletions that interfere with the kinase activity of the glucokinase but which do not significantly alter the three-dimensional structure of the domain are specifically contemplated by the invention.

5   Such crystalline polypeptides, or the atomic structure coordinates obtained therefrom, can be used to identify compounds that bind to the native domain. These compounds may affect the activity or the native domain.

The derivative crystals of the invention generally comprise a crystalline glucokinase

10   polypeptide in covalent association with one or more heavy metal atoms. The polypeptide may correspond to a native or a mutated Glucokinase. Heavy metal atoms useful for providing derivative crystals include, by way of example and not limitation, gold and mercury. Alternatively, derivative crystals can be formed from proteins which have heavy atoms incorporated into one or more amino acids, such as seleno-methionine

15   substitutions for methionine.

The co-crystals of the invention generally comprise a crystalline Glucokinase polypeptide in association with one or more compounds at an allosteric site of the polypeptide. The association may be covalent or non-covalent.

20   The native and mutated glucokinase polypeptides described herein may be isolated from natural sources or produced by methods well known to those skilled in the art of molecular biology. Expression vectors to be used may contain a native or mutated Glucokinase polypeptide coding sequence and appropriate transcriptional and/or translational control signals. These methods include in vitro recombinant DNA

25   techniques, synthetic techniques and in vivo recombination/genetic recombination. See, for example, the techniques described in Maniatis et al., 1989, *Molecular Cloning: A Laboratory Manual*, Cold Spring Harbor Laboratory, NY; and Ausubel et al., 1989, *Current Protocols in Molecular Biology*, Greene Publishing Associates and Wiley Interscience, NY.

30

- 5 -

A variety of host-expression vector systems may be utilized to express the Glucokinase coding sequence. These include but are not limited to microorganisms such as bacteria transformed with recombinant bacteriophage DNA, plasmid DNA or cosmid DNA expression vectors containing the Glucokinase coding sequence; yeast transformed

5   with recombinant yeast expression vectors containing the Glucokinase coding sequence; insect cell systems infected with recombinant virus expression vectors (e.g. baculovirus) containing the Glucokinase coding sequence; plant cell systems infected with recombinant virus expression vectors (e.g., cauliflower mosaic virus, CaMV; tobacco mosiac virus, TMV) or transformed with recombinant plasmid expression vectors (e.g., Ti

10   plasmid) containing the glucokinase coding sequence; or animal cell systems. The expression elements of these systems vary in their strength and specificities. Depending on the host/vector system utilized, any of a number of suitable transcription and translation elements, including constitutive and inducible promotors such as pL of bacteriophage μ, plac, ptrp, ptac (ptrp-lac hybrid promoter) and the like may be used;

15   when cloning in insect cell systems, promoters such as the baculovirus polyhedrin promoter may be used; when cloning in plant cell systems, promoters derived from the genome of plant cells (e.g., heat shock promoters; the promoter for the small subunit of RUBISCO; the promoter for the chlorophyll a/b binding protein) or from plant viruses (e.g., the 35 S RNA promoter of CaMV; the coat protein promoter of TMV) may be used;

20   when cloning in mammalian cell systems, promoters derived from the genome of mammalian cells (e.g., metallothionein promoter) or from mammalian viruses (e.g., the adenovirus late promoter; the vaccinia virus 7.5K promoter) may be used; when generating cell lines that contain multiple copies of the glucokinase coding sequence, SV40-, BPV- and EBV-based vectors may be used with an appropriate selectable marker.

25

The apo, derivative and co-crystals of the invention can be obtained by techniques well-known in the art of protein crystallography, including batch, liquid bridge, dialysis, vapor diffusion and hanging drop methods (see e.g. McPherson, 1982, *Preparation and Analysis of Protein Crystals*, John Wiley, NY; McPherson, 1990, *Eur. J. Biochem.* 189:1-23;

30   Webber, 1991, *Adv. Protein Chem.* 41:1-36; Crystallization of Nucleic Acids and Proteins, Edited by Arnaud Ducruix and Richard Giege, Oxford University Press; Protein Crystallization Techniques, Strategies, and Tips, Edited by Terese Bergfors, International University Line, 1999). Generally, the apo- or co-crystals of the invention are grown by

placing a substantially pure Glucokinase polypeptide in an aqueous buffer containing a precipitant at a concentration just below that necessary to precipitate the protein. Water is then removed from the solution by controlled evaporation to produce crystallizing conditions, which are maintained until crystal growth ceases.

5

In a preferred embodiment of the invention, apo or co-crystals are grown by vapor diffusion. In this method, the polypeptide/precipitant solution is allowed to equilibrate in a closed container with a larger aqueous reservoir having a precipitant concentration optimal for producing crystals. Generally, less than about 10 μL of subtantially pure

10   polypeptide solution is mixed with an equal volume of reservoir solution, giving a precipitant concentration about half that required for crystallization. This solution is suspended as a droplet underneath a coverslip, which is sealed onto the top of a reservoir. The sealed container is allowed to stand, from one day to one year, usually for about 2-6 weeks, until crystals grow.

15   For crystals of the invention, it has been found that hanging drops containing about 2-5 μl of Glucokinase (9-22 mg/ml in 20 mM tris pH 7.1 measured at room temperature, 50 mM NaCl, 50 mM glucose, 10 mM DTT and optionally 0.2 mM EDTA) and an equal amount of reservoir solution (16-25% w/v polyethylene glycol with an average molecular weight from about 8000 to about 10000 Daltons, 0.1-0.2 M tris or bistris or Hepes or

20   ammonium phosphate buffer, pH 6.9-7.5, 8-10 mM DTT, 0 - 30% saturated glucose) suspended over 0.5 to 1.0 mL reservoir buffer for about 3-4 weeks at 4-6°C provided crystals suitable for high resolution X-ray structure determination. Particularly preferred conditions were: about 2-5 μl of Glucokinase (10 mg/ml in 20 mM tris pH 7.1 measured at room temperature, 50 mM NaCl, 50 mM glucose, 10 mM DTT and optionally 0.2 mM

25   EDTA) and an equal amount of reservoir solution (22.5% w/v polyethylene glycol with an average molecular weight of about 10000 Daltons, 0.1 M tris pH 7.08, 10 mM DTT, 20% glucose) were suspended over 0.5 to 1.0 mL reservoir buffer for about 3-4 weeks at 4-6°C.

The optimum procedure for growing crystals large enough to collect data from involved first streaking 3-4 µl of protein solution on the coverslip, followed by streaking 3-4 µl of well solution across the elongated droplet of protein, forming a droplet shaped like the letter 'X'. Before discovering this crossed droplet technique, most droplets yielded

5   showers of small crystals which were not large enough for data collection purposes. The crossed droplets allow gradients of protein and precipitating agent to form as the two solutions slowly mix, and the resulting kinetics of crystal nucleation and growth are optimal for the growth of a small number of large crystals in each crossed droplet. Simply mixing the protein and precipitant solutions together in a single round droplet often

10   produced an overabundance of nuclei which grew to a final size too small for data collection purposes. Crystals usually appeared within 5 days of setup. The crystals grow in the form of hexagonal bipyramids, reaching dimensions of 0.2 x 0.2 x 0.4 mm typically, although larger crystals are often observed. Figure 1 shows grown crystals.

15   Crystals may be frozen prior to data collection. The crystals were cryo-protected with either (a) 20-30% saturated glucose present in the crystallization setup, (b) ethanol added to 15-20%, (c) ethylene glycol added to 10-20% and PEG10,000 brought up to 25%, or (d) glycerol added to 15%. The crystals were either briefly immersed in the cryo-protectant or soaked in the cryo-protectant for periods as long as a day. Freezing was

20   accomplished by immersing the crystal in a bath of liquid nitrogen or by placing the crystal in a stream of nitrogen gas at 100 K.

The mosaic spread of the frozen crystals could sometimes be reduced by annealing, wherein the stream of cold nitrogen gas is briefly blocked, allowing the frozen crystal to

25   thaw momentarily before re-freezing in the nitrogen gas stream. Another technique which was sometimes helpful in data collection was to center one of the ends of the hexagonal bipyramid in the x-ray beam, rather than the mid portion of the crystal. The mosaic spread could sometimes be reduced by this technique.

Diffraction data typically extending to 2.7 Å was collected from the frozen crystals at the synchrotron beamline X8C of the National Synchrotron Light Source in Brookhaven, New York. Under optimum conditions, data extending to 2.2 Å was recorded. See Figures 3 and 4 for solution. The space group of the crystals was determined to be

5   P6(5)22 during the course of the solution of the crystal structure. The crystals have unit cell dimensions a = b = 79.62 +/- 0.60 Å, c = 321.73 +/- 3.70 Å, $\alpha\gamma = \beta = 90°$, $\gamma = 120°$. The crystals are in a hexagonal system with P6(5)22 symmetry.

Of course, those having skill in the art will recognize that the above-described

10   crystallization conditions can be varied. Such variations may be used alone or in combination, and include polypeptide solutions containing polypeptide concentrations between 1 mg/mL and 60 mg/mL, any commercially available buffer systems which can maintain pH from about 6.5 to about 7.6, Tris-HCl concentrations between 10 mM and 200 mM, dithiothreitol concentrations between 0 mM and 20 mM, preferably between 8

15   and 10 mM, substitution of dithiothreitol with beta mercapto ethanol or other art-recognized equivalents, glucose concentrations between 0% w/v and 30% w/v, or substitution of glucose with other sugars known to bind to Glucokinase; and reservoir solutions containing polyethylene glycol (PEG) concentrations between about 10% and about 30%, polyethylene glycol average molecular weights between about 1000 and about

20   20,000 daltons, any commercially available buffer systems which can maintain pH from about 6.5 to about 7.6, dithiothreitol concentrations between 0 mM and 20 mM, substitution of dithiothreitol with beta mercapto ethanol or other art-recognized -SH group containing equivalents, or substitution of glucose with other sugars known to bind to Glucokinase, and temperature ranges between 4 and 20°C.

25

Derivative crystals of the invention can be obtained by soaking apo or co-crystals in mother liquor containing salts of heavy metal atoms, according to procedures known to those of skill in the art of X-ray crystallography.

Co-crystals of the invention can be obtained by soaking an apo crystal in mother liquor containing a ligand that binds to the allosteric site, or can be obtained by co-crystallizing the Glucokinase polypeptide in the presence of one or more ligands that bind to the allosteric site. Preferably, co-crystals are formed with a glucokinase activator disclosed in US Pat. No. 6,320,050; US Pat. Appl. 09/532,506 filed March 21, 2000; US Pat. Appl. 09/675,781 filed September 28, 2000; US Pat. Appl. 09/727,624, filed December 1, 2000; US Pat. Appl. 09/841,983, filed April 25, 2001; US Pat. Appl. 09/843,466, filed April 26, 2001; US Pat. Appl. 09/846,820, filed May 1, 2001; US Pat. Appl. 09/846,821, filed May 1, 2001; US Pat. Appl. 09/905,152, filed July 13, 2001; US Pat. Appl. 09/924,247, filed August 8, 2001; US Provisional Pat. Appl. 60/251,637, filed December 6, 2000; or US Provisional Pat. Appl. 60/318,715, filed September 13, 2001, each of which is incorporated herein by reference.

Methods for obtaining the three-dimensional structure of the crystalline glucokinases described herein, as well as the atomic structure coordinates, are well-known in the art (see, e.g., D. E. McRee, Practical Protein Crystallography, published by Academic Press, San Diego (1993), and references cited therein).

The crystals of the invention, and particularly the atomic structure coordinates obtained therefrom, have a wide variety of uses. For example, the crystals and structure coordinates described herein are particularly useful for identifying compounds that activate Glucokinases as an approach towards developing new therapeutic agents. One such compound is 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide and pharmaceutically acceptable salts thereof. Pharmaceutical compositions of said compounds can be developed, and said compounds can be used for the manufacture of a medicament comprising said compound for the treatment of hyperglycemia in type II diabetes.

The structure coordinates described herein can be used as phasing models in determining the crystal structures of additional native or mutated glucokinases, as well as

the structures of co-crystals of such glucokinases with allosteric inhibitors or activators bound. The structure coordinates, as well as models of the three-dimensional structures obtained therefrom, can also be used to aid the elucidation of solution-based structures of native or mutated glucokinases, such as those obtained via NMR. Thus, the crystals and

5   atomic structure coordinates of the invention provide a convenient means for elucidating the structures and functions of glucokinases.

For purposes of clarity and discussion, the crystals of the invention will be described by reference to specific Glucokinase exemplary apo crystals and co-crystals. Those skilled in the art will appreciate that the principles described herein are generally applicable to

10   crystals of any mammalian Glucokinase, including, but not limited to the Glucokinase of Figure 2.

As used herein, "allosteric site" refers in general to any ligand binding site on a mammalian Glucokinase other than the active site of the enzyme.

15

As used herein, "apo crystal" refers to crystals of mammalian Glucokinase formed without a bound allosteric ligand.

As used herein, "allosteric ligand" refers to any molecule which specifically binds an

20   allosteric site on a mammalian Glucokinase.

<u>EXAMPLES</u>

Example 1: Expression and Purification of Glucokinase

5 <u>Expression of GK</u>

Glucokinase (GK) was expressed as a glutathione S-transferase (GST) fusion protein in *Escherichia coli*. The amino-acid sequence of the fusion protein is given in Figure 2. The expression construct is based on the pGEX-3X vector from Pharmacia, as described

10 in Y. Liang, P. Kesavan, L. Wang, K. Niswender, Y. Tanizawa, M. A. Permutt, M. A. Magnuson, F. M. Matschinsky, *Biochem. J.* 309, 167 (1995). The construct codes for one of the two liver isozymes of human GK. The GST tag is at the N-terminus of the construct, and is separated from the coding sequence for GK by a Factor Xa cleavage site. After purification of the GST fusion protein, the GST fusion tag was removed with Factor

15 Xa protease, which also removes five residues from the N-terminus of GK.

<u>Purification of GK</u>

E. coli cells expressing GST-GK were suspended in lysis buffer (50 mM tris, 200 mM

20 NaCl, 5 mM EDTA, 5 mM DTT, 1% NP-40, pH 7.7) in the presence of protease inhibitors, incubated with lysozyme at 200 μ/ml for 30 minutes at room temperature, and sonicated 4x30 sec. at 4° C. After centrifugation to remove insoluble material, the supernatant was loaded onto glutathione-Sepharose, washed with lysis buffer and then with lysis buffer minus NP-40. GST-GK was eluted with lysis buffer (minus NP-40)

25 containing 50 mM D-glucose and 20 mM glutathione. The eluted protein was concentrated and dialyzed into 20 mM tris, 100 mM NaCl, 0.2 mM EDTA, 50 mM D-glucose, 1mM DTT, pH 7.7. Factor Xa was added at a protein ratio of 1:100 GST-GK followed by the addition of CaCl$_2$ to 1 mM, and the sample was incubated at 4° C for 48

hours. The sample was added to glutathione Sepharose and the unbound fraction collected and concentrated. The sample was then incubated with benzamidine Sepharose to remove Factor Xa, and the unbound fraction was collected and loaded on a Q Sepharose column equilibrated with 25 mM bis-tris propane, 50 mM NaCl, 5 mM DTT,

5   50 mM D-glucose and 5% glycerol (pH 7.0). The protein was eluted with a NaCl gradient from 50-400 mM. Fractions containing purified GK were pooled and concentrated and filtered.

Example 2: Formation of apo Crystal

10   4 μl of glucokinase and 4 μl of precipitant were mixed and equilibrated against the precipitant solution at 4° C.   The glucokinase solution consisted of 22 mg/ml glucokinase prepared in Example 1 in 20 mM hepes pH 7.5, 50 mM NaCl, 10 mM DTT, and 50 mM glucose. The precipitant consisted of 22.5% PEG10000, 0.1 M tris pH 7.08, 10 mM DTT, 20% glucose; the precipitant solution contained seed crystals in order to

15   microseed the droplets. Crystals appeared in the droplets after leaving the crystallization plates at 4° C.

Example 3: Formation of Co-crystal with 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide

20

3(a):

        4 μl of glucokinase and 4 μl of precipitant were mixed and equilibrated against the precipitant solution at 4° C.   The glucokinase solution consisted of 13 mg/ml glucokinase prepared in Example 1 in 20 mM tris pH 7.0, 50 mM NaCl, 10 mM DTT, 50 mM glucose,

25   and the glucokinase activator 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide at a concentration 5 times that of the protein. The precipitant consisted of 22.5% PEG10000, 0.1 M tris pH 7.08, 10 mM DTT, 20% glucose. Crystals appeared in the droplets after leaving the crystallization plates at 4° C.

3(b):

     Alternatively, crystals were grown as in Example 3(a) with the following changes: instead of 4 μl glucokinase and 4 μl precipitant, 2 μl of each were used; the glucokinase solution contained 11 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 22.5% PEG10000 as precipitant 18% PEG8000 was used; the precipitant solution contained seed crystals in order to microseed the droplets.

3(c):

     In another alternative, crystals were grown as in Example 3(a) with the following changes: instead of 4 μl glucokinase and 4 μl precipitant, 2 μl of each were used; the glucokinase solution contained 11 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 22.5% PEG10000 as precipitant 20% PEG8000 was used; the precipitant solution contained seed crystals in order to microseed the droplets.

3(d):

     In yet another alternative, crystals were grown as in Example 3(a) with the following changes: instead of 4 μl glucokinase and 4 μl precipitant, 2 μl of each were used; the glucokinase solution contained 12 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 22.5% PEG10000 as precipitant 16% PEG10000 was used; glucose was not present as a component of the precipitant; the precipitant solution contained seed crystals in order to microseed the droplets.

3(e):

     In still another alternative, crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 11 mg/ml glucokinase in tris

buffer at pH 7.1 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 22.5% PEG10000 as precipitant 25% PEG10000 was used.

3(f):

In still another alternative, crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 11 mg/ml glucokinase in tris buffer at pH 7.1 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 22.5% PEG10000 as precipitant 21.25% PEG10000 was used; in place of tris buffered at pH 7.08 in the precipitant tris buffered at pH 7.52 was used.

3(g):

In still another alternative, crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 12 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of tris buffered at pH 7.08 in the precipitant, hepes buffered at pH 6.89 was used; in place of 20% glucose in the precipitant, 200 mM glucose was used.

3(h):

In still another alternative, crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 12 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 0.1 M tris buffered at pH 7.08 in the precipitant, 0.2 M ammonium phosphate buffered at pH 7.03 was used; in place of 20% glucose in the precipitant, 200 mM glucose was used.

3(i):

In still another alternative, crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 10 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 22.5% PEG10000 as precipitant, 20% PEG10000 was used; in place of tris buffered at pH 7.08 in the precipitant, tris buffered at pH 7.05 was used; in place of 10 mM DTT in the precipitant, 8 mM DTT was used; glucose was not present as a component of the precipitant.

3(j):

In still another alternative, crystals were grown as in Example 3(a) with the
following changes: the glucokinase solution contained 12 mg/ml glucokinase in tris
5   buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place
of 22.5% PEG10000 as precipitant, 22% PEG8000 was used; glucose was not present as a
component of the precipitant; the precipitant solution contained seed crystals in order to
microseed the droplets.

3(k):

10   In still another alternative, crystals were grown as in Example 3(a) with the
following changes: the glucokinase solution contained 11 mg/ml glucokinase in tris
buffer at pH 7.1 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place
of 20% glucose in the precipitant, 30% glucose was used.

15   **Example 4: Formation of Co-crystal with N-(5-Bromo-pyridin-2-yl)-2-(3-chloro-4-
methanesulfonyl-phenyl)-3-cyclopentyl-propionamide**

Crystals were grown as in Example 3(a) with the following changes: the
glucokinase solution contained 9 mg/ml glucokinase in tris buffer at pH 7.1 instead of
20   7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase
activator of Example 3(a), the glucokinase solution contained the glucokinase activator
N-(5-Bromo-pyridin-2-yl)-2-(3-chloro-4-methanesulfonyl-phenyl)-3-cyclopentyl-
propionamide; in place of 20% glucose in the precipitant, 200 mM glucose was used.

25   **Example 5: Formation of Co-crystal with 2-(3-Chloro-4-methanesulfonyl-phenyl)-3-
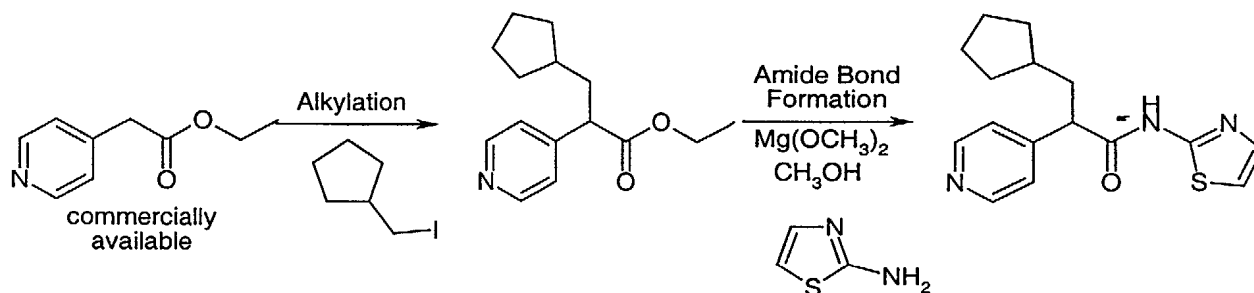cyclopentyl-N-(5-trifluoromethyl-pyridin-2-yl)-propionamide**

Crystals were grown as in Example 3(a) with the following changes: the
glucokinase solution contained 10 mg/ml glucokinase in tris buffer at pH 7.1 instead of
30   7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase

activator of Example 3(a), the glucokinase solution contained the glucokinase activator 2-(3-Chloro-4-methanesulfonyl-phenyl)-3-cyclopentyl-N-(5-trifluoromethyl-pyridin-2-yl)-propionamide; in place of 22.5% PEG10000 as precipitant, 21.25% PEG10000 was used.

Example 6: Formation of Co-crystal with (2S)-2-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionylamino]-thiazole-4-carboxylic acid methyl ester

Crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 10 mg/ml glucokinase in tris buffer at pH 7.1 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase activator of Example 3(a), the glucokinase solution contained the glucokinase activator (2S)-2-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionylamino]-thiazole-4-carboxylic acid methyl ester; in place of 22.5% PEG10000 as precipitant, 21.25% PEG10000 was used; in place of tris buffered at pH 7.08 in the precipitant, bistris buffered at pH 7.0 was used.

Example 7: Formation of Co-crystal with (2S)-{2-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionylamino]-thiazol-5-yl}-oxo-acetic acid ethyl ester

Crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 10 mg/ml glucokinase in tris buffer at pH 7.1 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase activator of Example 3(a), the glucokinase solution contained the glucokinase activator (2S)-{2-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionylamino]-thiazol-5-yl}-oxo-acetic acid ethyl ester; in place of 22.5% PEG10000 as precipitant, 21.25% PEG10000 was used.

Example 8: Formation of Co-crystal with (2S)-{3-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionyl]-ureido}-acetic acid methylester

Crystals were grown as in Example 3(a) with the following changes: the
glucokinase solution contained 9 mg/ml glucokinase in tris buffer at pH 7.08 instead of
7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase
activator of Example 3(a), the glucokinase solution contained the glucokinase activator
(2S)-{3-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionyl]-ureido}-acetic acid
methylester; in place of 20% glucose in the precipitant, 200 mM glucose was used.

Example 9: Formation of Co-crystal with (2S)-1-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionyl]-3-(3-hydroxy-propyl)-urea

Crystals were grown as in Example 3(a) with the following changes: the
glucokinase solution contained 14 mg/ml glucokinase in tris buffer at pH 7.08 instead of
7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase
activator of Example 3(a), the glucokinase solution contained the glucokinase activator
(2S)-1-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionyl]-3-(3-hydroxy-propyl)-urea; in
place of 20% glucose in the precipitant, 200 mM glucose was used.

Example 10: Formation of Co-crystal with (2S)-{3-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionyl]-ureido}-acetic acid ethyl ester

Crystals were grown as in Example 3(a) with the following changes: the
glucokinase solution contained 14 mg/ml glucokinase in tris buffer at pH 7.08 instead of
7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase
activator of Example 3(a), the glucokinase solution contained the glucokinase activator
(2S)-{3-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionyl]-ureido}-acetic acid ethyl
ester; in place of tris buffered at pH 7.08 in the precipitant, tris buffered at pH 7.05 was
used.

Example 11: Synthesis of 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide

3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide can be prepared using well-

known organic synthesis techniques according to the following reaction scheme:

5   3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide is useful as an

allosteric activator of Glucokinase and to assist the formation of co-crystals of

Glucokinase.

In the present specification "comprises" means "includes or consists of" and "comprising" means "including or consisting of".

5   The features disclosed in the foregoing description, or the following claims, or the accompanying drawings, expressed in their specific forms or in terms of a means for performing the disclosed function, or a method or process for attaining the disclosed result, as appropriate, may, separately, or in any combination of such features, be utilised for realising the invention in diverse

10   forms thereof.

SEQUENCE LISTING

<110>   F. Hoffmann - La Roche

<120>   CRYSTALS OF GLUCOKINASE AND METHODS OF GROWING THEM

<130>   Case 20892

<140>   US 60/341988

<141>   2001-12-19

<150>   US 60/341988

<151>   2001-12-19

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<309>   1994-12-13

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Tyr Glu Arg Asp Glu Gly Asp Lys Trp Arg Asn Lys Lys Phe Glu Leu

21

Gly Leu Glu Phe Pro Asn Leu Pro Tyr Tyr Ile Asp Gly Asp Val Lys

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Leu Thr Gln Ser Met Ala Ile Ile Arg Tyr Ile Ala Asp Lys His Asn

5   65   70   75   80

Met Leu Gly Gly Cys Pro Lys Glu Arg Ala Glu Ile Ser Met Leu Glu

85   90   95

Gly Ala Val Leu Asp Ile Arg Tyr Gly Val Ser Arg Ile Ala Tyr Ser

100   105   110

10 Lys Asp Phe Glu Thr Leu Lys Val Asp Phe Leu Ser Lys Leu Pro Glu

115   120   125

Met Leu Lys Met Phe Glu Asp Arg Leu Cys His Lys Thr Tyr Leu Asn

130   135   140

Gly Asp His Val Thr His Pro Asp Phe Met Leu Tyr Asp Ala Leu Asp

15 145   150   155   160

Val Val Leu Tyr Met Asp Pro Met Cys Leu Asp Ala Phe Pro Lys Leu

165   170   175

Val Cys Phe Lys Lys Arg Ile Glu Ala Ile Pro Gln Ile Asp Lys Tyr

180   185   190

20 Leu Lys Ser Ser Lys Tyr Ile Ala Trp Pro Leu Gln Gly Trp Gln Ala

195   200   205

Thr Phe Gly Gly Gly Asp His Pro Pro Lys Ser Asp Leu Ile Glu Gly

210   215   220

Arg Gly Ile His Met Pro Arg Pro Arg Ser Gln Leu Pro Gln Pro Asn

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Ser Gln Val Glu Gln Ile Leu Ala Glu Phe Gln Leu Gln Glu Glu Asp

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Leu Lys Lys Val Met Arg Arg Met Gln Lys Glu Met Asp Arg Gly Leu

Arg Leu Glu Thr His Glu Glu Ala Ser Val Lys Met Leu Pro Thr Tyr

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Val Arg Ser Thr Pro Glu Gly Ser Glu Val Gly Asp Phe Leu Ser Leu

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Asp Leu Gly Gly Thr Asn Phe Arg Val Met Leu Val Lys Val Gly Glu

305   310   315   320

Gly Glu Glu Gly Gln Trp Ser Val Lys Thr Lys His Gln Met Tyr Ser

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20 Lys Arg Arg Gly Asp Phe Glu Met Asp Val Val Ala Met Val Asn Asp

              420   425   430

Thr Val Ala Thr Met Ile Ser Cys Tyr Tyr Glu Asp His Gln Cys Glu

              435   440   445

Val Gly Met Ile Val Gly Thr Gly Cys Asn Ala Cys Tyr Met Glu Glu

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Met Gln Asn Val Glu Leu Val Glu Gly Asp Glu Gly Arg Met Cys Val

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Cys Ser Ala Gly Leu Ala Gly Val Ile Asn Arg Met Arg Glu Ser Arg

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Met Leu Gly Gln

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        690
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1. A co-crystal of mammalian Glucokinase and a ligand bound to an allosteric site of the Glucokinase, wherein

   the co-crystal has unit cell dimensions of:

   a and b are from 79.02 Å to 80.22 Å;

   c is from 318.03 Å to 325.03 Å;

   α and β are 90°; and

   γ is 120°;

   and the co-crystal has P6(5)22 symmetry.

2. A crystal of mammalian Glucokinase, wherein

   the crystal has unit cell dimensions of:

   a and b are from 79.02 Å to 80.22 Å;

   c is from 318.03 Å to 325.03 Å;

   α and β are 90°; and

   γ is 120°;

   and the crystal has P6(5)22 symmetry.

3. A process for co-crystalizing mammalian Glucokinase and an allosteric ligand of Glucokinase, the process comprising:

   providing a buffered, aqueous solution of 9 to 22 mg/ml of the mammalian Glucokinase;

adding a molar excess of the allosteric ligand to the aqueous solution of mammalian Glucokinase; and

growing crystals by vapor diffusion using a buffered reservoir solution between about 10% and about 30% PEG, about 0% w/v and about 30% w/v glucose, and between 0 and 20 mM DTT, wherein the PEG has an average molecular weight between about 1,000 and about 20,000.

4. The process of claim 3, wherein the step of growing crystals by vapor diffusion comprises:

streaking the buffered, aqueous solution of mammalian Glucokinase with added allosteric ligand on a surface to form an elongated droplet of protein solution, and

streaking about an equal amount of the buffered reservoir solution across the elongated droplet of protein solution, forming a combined droplet shaped like the letter 'X'.

5. A crystal produced by the process of claims 3 or 4.

6. A compound identified by analysing the structure coordinates of the co-crystal of claim 1, said compound being a ligand that binds to the allosteric site of Glucokinase.
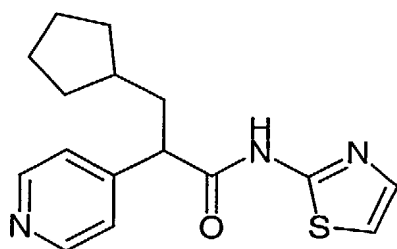
7. The compound

and pharmaceutically acceptable salts thereof.

8. A pharmaceutical composition comprising the compound of claim 6.

5

9. The pharmaceutical composition of claim 8, wherein said compound is the compound of claim 7.

10. Use of the compound of claim 6 for the manufacture of a medicament comprising a compound according to claim 6 for the treatment of hyperglycemia in type II diabetes.

11. The use of claim 10 wherein said compound is the compound of claim 7.

15 12. A compound according to claims 6 or 7, for use as a therapeutic active substance, in particular for the reduction of hyperglycemia in type II diabetes.

13. The novel crystals, processes, compounds, compositions and uses as hereinbefore described.

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27

14.   A process according to Claim 3 or 4 further comprising the step of freezing the crystals.

15.   A method of identifying a ligand that binds to the allosteric site of Glucokinase comprising analysing the structure co-ordinates of a co-crystal according to Claim 1.

16.   Use of a co-crystal according to Claim 1 or a crystal according to Claim 2 in the identification of a compound which activates Glucokinase.

17.   Use of a co-crystal according to Claim 1 or a crystal according to Claim 2 for elucidating the structure and function of a Glucokinase.

18.   A compound according to Claim 6 or 7, or a composition according to Claim 8 or 9, for use in a method of treatment of human or animal body.

19.   Any novel feature or combination of features described herein.

Application No: GB 0229456.9 **Examiner:** Dr Rowena Dinham
Claims searched: 1-5 & 14-17; and 12, 13, 18 **Date of search:** 16 June 2003
and 19 (in part)

Patents Act 1977 : Search Report under Section 17

Documents considered to be relevant:

Category	Relevant to claims	Identity of document and passage or figure of particular relevance
A, P		*Protein Science*; Vol 11, pp 2456-2463 (2002). Tsuge *et al.* "*Crystal structure of the ADP-dependent glucokinase...*" See entire document, especially Results and Discussion "*Overall strucure*"
A		*Structure*; Vol 9, pp 205-214 (2001). Ito *et al.* "*Structural basis for the ADP-specificity of a novel glucokinase...*" See entire document, especially Results and Discussion "*Crystal structure of* T. lioralis *glucokinase*"
A		*Diabetes*; Vol 48, pp 1698-1705 (1999). Mahalingam *et al.* "*Structural model of human glucokinase...*" See entire document, especially Results "*Overall model and comparison with previous model and hexokinase structures*"

Categories:

X	Document indicating lack of novelty or inventive step	A	Document indicating technological background and/or state of the art.
Y	Document indicating lack of inventive step if combined with one or more other documents of same category.	P	Document published on or after the declared priority date but before the filing date of this invention.
&	Member of the same patent family	E	Patent document published on or after, but with priority date earlier than, the filing date of this application.

Field of Search:

Search of GB, EP, WO & US patent documents classified in the following areas of the UKC^V:

Worldwide search of patent documents classified in the following areas of the IPC^7:

C12N; C30B; G06F

The following online and other databases have been used in the preparation of this search report:

WPI, EPODOC, JAPIO, MEDLINE, BIOSIS, EMBASE, SCISEARCH, CAPLUS